

## STN Search

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	APR 02	CAS Registry Number Crossover Limits Increased to 500,000 in Key STN Databases
NEWS	3	APR 02	PATDPAFULL: Application and priority number formats enhanced
NEWS	4	APR 02	DWPI: New display format ALLSTR available
NEWS	5	APR 02	New Thesaurus Added to Derwent Databases for Smooth Sailing through U.S. Patent Codes
NEWS	6	APR 02	EMBASE Adds Unique Records from MEDLINE, Expanding Coverage back to 1948
NEWS	7	APR 07	CA/CAplus CLASS Display Streamlined with Removal of Pre-IPC 8 Data Fields
NEWS	8	APR 07	50,000 World Traditional Medicine (WTM) Patents Now Available in CAplus
NEWS	9	APR 07	MEDLINE Coverage Is Extended Back to 1947
NEWS	10	JUN 16	WPI First View (File WPIFV) will no longer be available after July 30, 2010
NEWS	11	JUN 18	DWPI: New coverage - French Granted Patents
NEWS	12	JUN 18	CAS and FIZ Karlsruhe announce plans for a new STN platform
NEWS	13	JUN 18	IPC codes have been added to the INSPEC backfile (1969-2009)
NEWS	14	JUN 21	Removal of Pre-IPC 8 data fields streamline displays in CA/CAplus, CASREACT, and MARPAT
NEWS	15	JUN 21	Access an additional 1.8 million records exclusively enhanced with 1.9 million CAS Registry Numbers -- EMBASE Classic on STN
NEWS	16	JUN 28	Introducing "CAS Chemistry Research Report": 40 Years of Biofuel Research Reveal China Now Atop U.S. in Patenting and Commercialization of Bioethanol
NEWS	17	JUN 29	Enhanced Batch Search Options in DGENE, USGENE, and PCTGEN
NEWS	18	JUL 19	Enhancement of citation information in INPADOC databases provides new, more efficient competitor analyses
NEWS	19	JUL 26	CAS coverage of global patent authorities has expanded to 61 with the addition of Costa Rica
NEWS	EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2, AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.		
NEWS HOURS		STN Operating Hours Plus Help Desk Availability	

## Updated Search

## STN Search

NEWS LOGIN      Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 17:40:37 ON 05 AUG 2010

=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE  
ENTRY  
TOTAL  
SESSION  
0.22  
0.22  
FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:40:47 ON 05 AUG 2010  
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STRUCTURE FILE UPDATES: 4 AUG 2010 HIGHEST RN 1235013-90-7  
DICTIONARY FILE UPDATES: 4 AUG 2010 HIGHEST RN 1235013-90-7

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TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Documents and Settings\brobinson1\My Documents\aeerararare.str

## L1 STRUCTURE UPLOADED

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=> s 11
SAMPLE SEARCH INITIATED 17:44:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12433 TO ITERATE
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16.1% PROCESSED 2000 ITERATIONS

50 ANSWERS

## Updated Search

STN Search

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 241977 TO 255343  
PROJECTED ANSWERS: 22631 TO 26851

L2 50 SEA SSS SAM L1

=> s 11 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 191.05 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 17:44:44 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 246228 TO ITERATE

100.0% PROCESSED 246228 ITERATIONS 22969 ANSWERS  
SEARCH TIME: 00.00.01

L3 22969 SEA SSS FUL L1

=> file hcaplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
SESSION  
FULL ESTIMATED COST ENTRY 194.48 194.70

FILE 'HCAPLUS' ENTERED AT 17:44:48 ON 05 AUG 2010  
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FILE COVERS 1907 - 5 Aug 2010 VOL 153 ISS 6  
FILE LAST UPDATED: 4 Aug 2010 (20100804/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

Updated Search

STN Search

=> s 13  
L4 5489 L3

=> s 14 and jernstedt, h?/au  
3 JERNSTEDT, H?/AU  
L5 1 L4 AND JERNSTEDT, H?/AU

=> d 15, ibib abs fhitstr, 1  
THE ESTIMATED COST FOR THIS REQUEST IS 5.81 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2005:409459 HCAPLUS  
DOCUMENT NUMBER: 142:463609  
TITLE: Preparation of [(phenyl/pyridinyl)amino]alkanols and related compounds as androgen receptor modulators with therapeutic uses  
INVENTOR(S): Jernstedt, Henrik; Garg, Neeraj; Gustavsson, Annika; Gillner, Mikael; Garcia Collazo, Ana Maria; Koch, Eva  
PATENT ASSIGNEE(S): Karo Bio AB, Swed.; Elsy, David  
SOURCE: PCT Int. Appl., 98 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

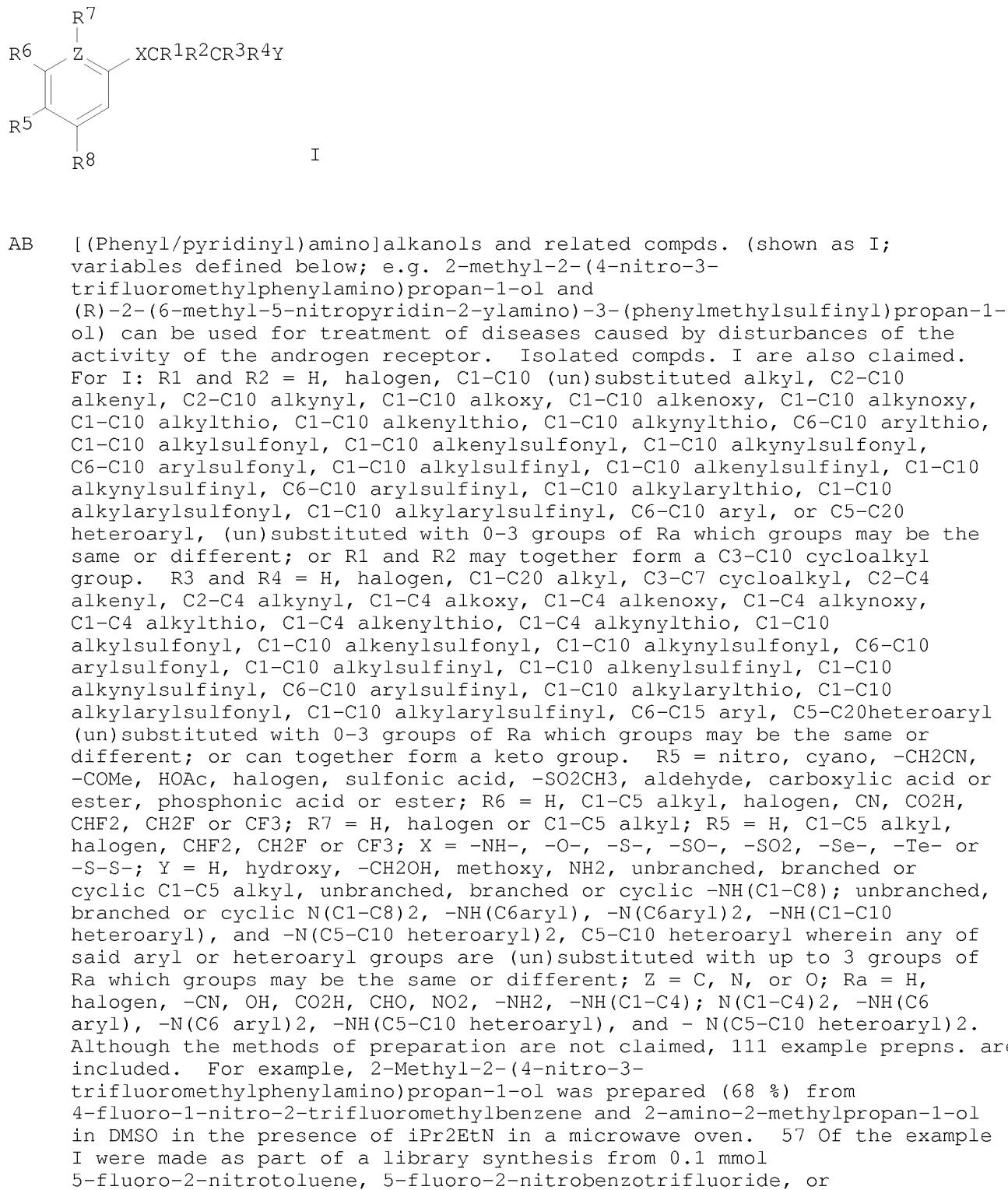
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004285744	A1	20050512	AU 2004-285744	20041021
CA 2543345	A1	20050512	CA 2004-2543345	20041021
EP 1685090	A1	20060802	EP 2004-768980	20041021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007509116	T	20070412	JP 2006-536167	20041021
IN 2006KN01357	A	20070504	IN 2006-KN1357	20060522
US 20080058383	A1	20080306	US 2007-576777	20070612
PRIORITY APPLN. INFO.:			GB 2003-24551	A 20031021
			WO 2004-GB4464	W 20041021

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 142:463609; MARPAT 142:463609

GI

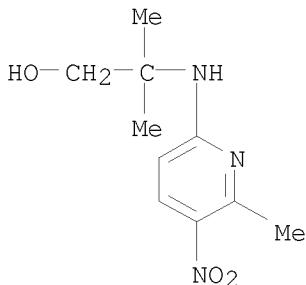
Updated Search



## STN Search

6-fluoro-2-methyl-3-nitropyridine in a vial to which was added 0.5 mL DMSO, 20  $\mu$ L triethylamine (1.4 equiv), and 1.4 equiv of 1 of many diverse amino alcs. and the vials were heated in a microwave oven. Androgen receptor competition binding and transactivation (agonist and antagonist) assay results are tabulated for 14 examples of I.

IT 353285-92-4P, 2-Methyl-2-(6-methyl-5-nitropyridin-2-ylamino)propan-1-ol  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (drug candidate; preparation of [(phenyl/pyridinyl)amino]alkanols and related compds. as androgen receptor modulators with therapeutic uses)  
 RN 353285-92-4 HCAPLUS  
 CN 1-Propanol, 2-methyl-2-[(6-methyl-5-nitro-2-pyridinyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
 (4 CITINGS)  
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 17:40:37 ON 05 AUG 2010)

FILE 'REGISTRY' ENTERED AT 17:40:47 ON 05 AUG 2010

L1 STRUCTURE uploaded  
 L2 50 S L1  
 L3 22969 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 17:44:48 ON 05 AUG 2010

L4 5489 S L3  
 L5 1 S L4 AND JERNSTEDT, H?/AU

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.45	212.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.85	-0.85

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STRUCTURE FILE UPDATES: 4 AUG 2010 HIGHEST RN 1235013-90-7  
DICTIONARY FILE UPDATES: 4 AUG 2010 HIGHEST RN 1235013-90-7

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Documents and Settings\brobinson1\My Documents\ataraatatatatat.str

L6 STRUCTURE UPLOADED

=> s 16  
SAMPLE SEARCH INITIATED 17:47:11 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 455 TO ITERATE

100.0% PROCESSED 455 ITERATIONS 12 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7821 TO 10379  
PROJECTED ANSWERS: 33 TO 447

L7 12 SEA SSS SAM L6

=> s 16 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 191.05 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 17:47:16 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 8926 TO ITERATE

100.0% PROCESSED 8926 ITERATIONS 186 ANSWERS  
SEARCH TIME: 00.00.01

L8 186 SEA SSS FUL L6

Updated Search

STN Search

=> file hcplus			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
	ENTRY	SESSION	
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
	ENTRY	SESSION	
CA SUBSCRIBER PRICE	0.00	-0.85	

FILE 'HCAPLUS' ENTERED AT 17:47:20 ON 05 AUG 2010  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 5 Aug 2010 VOL 153 ISS 6  
FILE LAST UPDATED: 4 Aug 2010 (20100804/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2010  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2010

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 18  
L9 95 L8

=> s 19 and jernstedt, h?/au  
3 JERNSTEDT, H?/AU  
L10 1 L9 AND JERNSTEDT, H?/AU

=> d 110, ibib abs fhitstr, 1  
THE ESTIMATED COST FOR THIS REQUEST IS 5.81 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2005:409459 HCAPLUS  
DOCUMENT NUMBER: 142:463609  
TITLE: Preparation of [(phenyl/pyridinyl)amino]alkanols and related compounds as androgen receptor modulators with

Updated Search

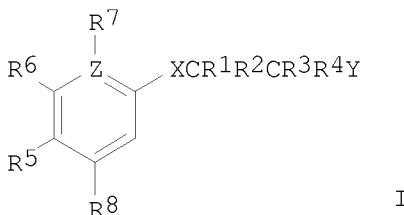
therapeutic uses  
 INVENTOR(S): Jernstedt, Henrik; Garg, Neeraj; Gustavsson, Annika; Gillner, Mikael; Garcia Collazo, Ana Maria; Koch, Eva  
 PATENT ASSIGNEE(S): Karo Bio AB, Swed.; Elsy, David  
 SOURCE: PCT Int. Appl., 98 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005042464	A1	20050512	WO 2004-GB4464	20041021
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004285744	A1	20050512	AU 2004-285744	20041021
CA 2543345	A1	20050512	CA 2004-2543345	20041021
EP 1685090	A1	20060802	EP 2004-768980	20041021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007509116	T	20070412	JP 2006-536167	20041021
IN 2006KN01357	A	20070504	IN 2006-KN1357	20060522
US 20080058383	A1	20080306	US 2007-576777	20070612
PRIORITY APPLN. INFO.:			GB 2003-24551	A 20031021
			WO 2004-GB4464	W 20041021

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 142:463609; MARPAT 142:463609

GI



AB [(Phenyl/pyridinyl)amino]alkanols and related compds. (shown as I; variables defined below; e.g. 2-methyl-2-(4-nitro-3-trifluoromethylphenylamino)propan-1-ol and (R)-2-(6-methyl-5-nitropyridin-2-ylamino)-3-(phenylmethylsulfinyl)propan-1-

ol) can be used for treatment of diseases caused by disturbances of the activity of the androgen receptor. Isolated compds. I are also claimed. For I: R1 and R2 = H, halogen, C1-C10 (un)substituted alkyl, C2-C10 alkenyl, C2-C10 alkynyl, C1-C10 alkoxy, C1-C10 alkenoxy, C1-C10 alkynoxy, C1-C10 alkylthio, C1-C10 alkenylthio, C1-C10 alkynylthio, C6-C10 arylthio, C1-C10 alkylsulfonyl, C1-C10 alkenylsulfonyl, C1-C10 alkynylsulfonyl, C6-C10 arylsulfonyl, C1-C10 alkylsulfinyl, C1-C10 alkenylsulfinyl, C1-C10 alkynylsulfinyl, C6-C10 arylsulfinyl, C1-C10 alkylarylylthio, C1-C10 alkylarylsulfonyl, C1-C10 alkylarylsulfinyl, C6-C10 aryl, or C5-C20 heteroaryl, (un)substituted with 0-3 groups of Ra which groups may be the same or different; or R1 and R2 may together form a C3-C10 cycloalkyl group. R3 and R4 = H, halogen, C1-C20 alkyl, C3-C7 cycloalkyl, C2-C4 alkenyl, C2-C4 alkynyl, C1-C4 alkoxy, C1-C4 alkenoxy, C1-C4 alkynoxy, C1-C4 alkylthio, C1-C4 alkenylthio, C1-C4 alkynylthio, C1-C10 alkylsulfonyl, C1-C10 alkenylsulfonyl, C1-C10 alkynylsulfonyl, C6-C10 arylsulfonyl, C1-C10 alkylsulfinyl, C1-C10 alkenylsulfinyl, C1-C10 alkynylsulfinyl, C6-C10 arylsulfinyl, C1-C10 alkylarylylthio, C1-C10 alkylarylsulfonyl, C1-C10 alkylarylsulfinyl, C6-C15 aryl, C5-C20heteroaryl (un)substituted with 0-3 groups of Ra which groups may be the same or different; or can together form a keto group. R5 = nitro, cyano, -CH2CN, -COMe, HOAc, halogen, sulfonic acid, -SO2CH3, aldehyde, carboxylic acid or ester, phosphonic acid or ester; R6 = H, C1-C5 alkyl, halogen, CN, CO2H, CHF2, CH2F or CF3; R7 = H, halogen or C1-C5 alkyl; R5 = H, C1-C5 alkyl, halogen, CHF2, CH2F or CF3; X = -NH-, -O-, -S-, -SO-, -SO2, -Se-, -Te- or -S-S-; Y = H, hydroxy, -CH2OH, methoxy, NH2, unbranched, branched or cyclic C1-C5 alkyl, unbranched, branched or cyclic -NH(C1-C8); unbranched, branched or cyclic N(C1-C8)2, -NH(C6aryl), -N(C6aryl)2, -NH(C1-C10 heteroaryl), and -N(C5-C10 heteroaryl)2, C5-C10 heteroaryl wherein any of said aryl or heteroaryl groups are (un)substituted with up to 3 groups of Ra which groups may be the same or different; Z = C, N, or O; Ra = H, halogen, -CN, OH, CO2H, CHO, NO2, -NH2, -NH(C1-C4); N(C1-C4)2, -NH(C6 aryl), -N(C6 aryl)2, -NH(C5-C10 heteroaryl), and -N(C5-C10 heteroaryl)2. Although the methods of preparation are not claimed, 111 example preps. are included. For example, 2-Methyl-2-(4-nitro-3-trifluoromethylphenylamino)propan-1-ol was prepared (68 %) from 4-fluoro-1-nitro-2-trifluoromethylbenzene and 2-amino-2-methylpropan-1-ol in DMSO in the presence of iPr2EtN in a microwave oven. 57 Of the example I were made as part of a library synthesis from 0.1 mmol 5-fluoro-2-nitrotoluene, 5-fluoro-2-nitrobenzotrifluoride, or 6-fluoro-2-methyl-3-nitropyridine in a vial to which was added 0.5 mL DMSO, 20  $\mu$ L triethylamine (1.4 equiv), and 1.4 equiv of 1 of many diverse amino alcs. and the vials were heated in a microwave oven. Androgen receptor competition binding and transactivation (agonist and antagonist) assay results are tabulated for 14 examples of I.

IT 851445-91-5P, (S)-2-(4-Nitro-3-trifluoromethylphenylamino)butan-1-ol

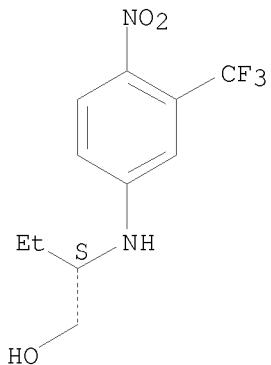
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of [(phenyl/pyridinyl)amino]alkanols and related compds. as androgen receptor modulators with therapeutic uses)

RN 851445-91-5 HCAPLUS

CN 1-Butanol, 2-[(4-nitro-3-(trifluoromethyl)phenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
 (4 CITINGS)  
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 17:40:37 ON 05 AUG 2010)

FILE 'REGISTRY' ENTERED AT 17:40:47 ON 05 AUG 2010

L1 STRUCTURE uploaded  
 L2 50 S L1  
 L3 22969 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 17:44:48 ON 05 AUG 2010

L4 5489 S L3  
 L5 1 S L4 AND JERNSTEDT, H?/AU

FILE 'REGISTRY' ENTERED AT 17:46:57 ON 05 AUG 2010

L6 STRUCTURE uploaded  
 L7 12 S L6  
 L8 186 S L6 FULL

FILE 'HCAPLUS' ENTERED AT 17:47:20 ON 05 AUG 2010

L9 95 S L8  
 L10 1 S L9 AND JERNSTEDT, H?/AU

=> s l9 not l10  
 L11 94 L9 NOT L10

=> s l11 and garg, n?/au  
 364 GARG, N?/AU  
 L12 0 L11 AND GARG, N?/AU

=> s l11 and gustavsson, a?/au  
 172 GUSTAVSSON, A?/AU  
 L13 0 L11 AND GUSTAVSSON, A?/AU

=> s l11 and gillner, m?/au

STN Search

L14 64 GILLNER, M?/AU  
0 L11 AND GILLNER, M?/AU

=> s l11 and collazo, a?/au  
44 COLLAZO, A?/AU  
L15 0 L11 AND COLLAZO, A?/AU

=> s l11 and koch, e?/au  
1206 KOCH, E?/AU  
L16 0 L11 AND KOCH, E?/AU

=> d l11, ibib abs fhitstr, 1-94  
THE ESTIMATED COST FOR THIS REQUEST IS 546.14 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L11 ANSWER 1 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2009:846111 HCPLUS  
DOCUMENT NUMBER: 151:92848  
TITLE: Method using lifespan-altering compounds for altering  
the lifespan of eukaryotic organisms, and screening  
for such compounds  
INVENTOR(S): Goldfarb, David Scott  
PATENT ASSIGNEE(S): University of Rochester, USA  
SOURCE: U.S. Pat. Appl. Publ., 57pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 20  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
AU 2008345225	A1	20090709	AU 2008-345225	20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P 20080125
			US 2007-16362P	P 20071221
			US 2008-341615	20081222
			WO 2008-US88016	W 20081222

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

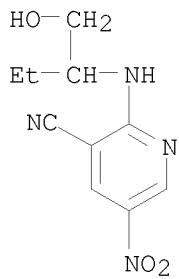
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 180424-16-2

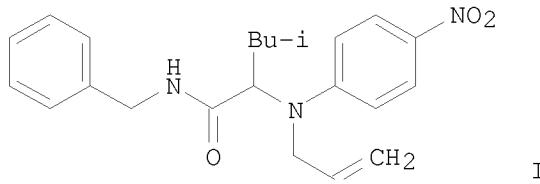
RL: PAC (Pharmacological activity); BIOL (Biological study)  
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 180424-16-2 HCPLUS

CN 3-Pyridinecarbonitrile, 2-[(1-(hydroxymethyl)propyl]amino]-5-nitro- (CA INDEX NAME)



L11 ANSWER 2 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2009:770529 HCPLUS  
 DOCUMENT NUMBER: 151:245287  
 TITLE: Isocyanide-based multicomponent reaction 'without' isocyanides  
 AUTHOR(S): El Kaim, Laurent; Grimaud, Laurence; Schiltz, Aurelie  
 CORPORATE SOURCE: Laboratoire Chimie et Procedes, Ecole Nationale Superieure de Techniques Avancees, Paris, 75739/15, Fr.  
 SOURCE: Synlett (2009), (9), 1401-1404  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 151:245287  
 GI



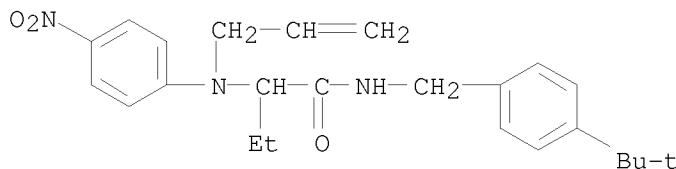
AB We present here a one-pot, four-component sequence that affords Ugi-type adducts, e.g., I, starting from simple benzyl or allyl bromides. The isocyanides are prepared in situ under alkylation of silver cyanide salts and the resulting mixture is directly used in a Ugi-Smiles coupling.

IT 1178564-05-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of amino amide derivs. via isocyanation of benzylbromides with cyanides followed by Ugi-Smiles coupling with nitrophenols, amines and aldehydes)

RN 1178564-05-0 HCPLUS

CN Butanamide, N-[(4-(1,1-dimethylethyl)phenyl)methyl]-2-[(4-nitrophenyl)-2-propen-1-ylamino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)  
 REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:659155 HCAPLUS

DOCUMENT NUMBER: 151:221431

TITLE: Analysis of multicomponent mixture and simultaneous enantioresolution of proteinogenic and non-proteinogenic amino acids by reversed-phase high-performance liquid chromatography using chiral variants of Sanger's reagent

AUTHOR(S): Bhushan, Ravi; Kumar, Rajender

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, 247 667, India

SOURCE: Analytical and Bioanalytical Chemistry (2009), 394(6), 1697-1705

CODEN: ABCNBP; ISSN: 1618-2642

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:221431

AB Four chiral derivatizing reagents (CDR), namely, FDNP-L-Ala, FDNP-L-Val, FDNP-L-Phe, and FDNP-L-Leu, were synthesized using microwave (MW) irradiation by substituting one of the fluorine atoms in difluoro dinitro benzene (DFDNB) with L-Ala, L-Val, L-Phe, and L-Leu. The other set of CDRs, namely, FDNP-L-Phe-NH<sub>2</sub>, FDNP-L-Val-NH<sub>2</sub>, and FDNP-L-Leu-NH<sub>2</sub>, was also prepared. These reagents were used for synthesis of diastereomers of 18 proteinogenic and 8 non-proteinogenic amino acids, which were resolved by reversed-phase high-performance liquid chromatog. using C18 column and gradient eluting mixture of aqueous TFA and acetonitrile with UV detection at 340 nm. The reagents were used for resolution of a complex mixture of 18 racemic proteinogenic amino acids in a single chromatog. run of 65 min and to determine concentration of the D-amino acid in a solution of DL-amino acid.

The

resolution (Rs) and selectivity ( $\alpha$ ) obtained for the two sets of diastereomers were compared among themselves and among the two groups. The method was validated for accuracy, precision, limit of detection (LOD), and limit of quantification. LOD is 0.001% impurity of D-enantiomer.

IT 1122591-18-7P

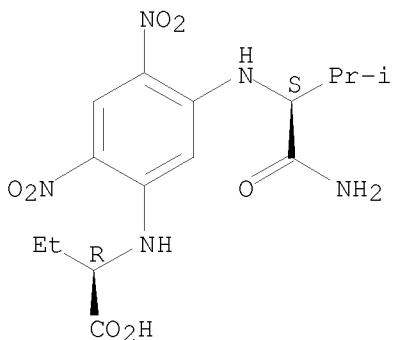
RL: ANT (Analyte); PUR (Purification or recovery); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
 (synthesis of Sanger chiral derivatizing reagents by fluorine substitution in difluoro dinitro benzene with amino acid under microwave irradiation and their using for enantiomeric resolution of amino acids by reversed-phase HPLC)

STN Search

RN 1122591-18-7 HCPLUS

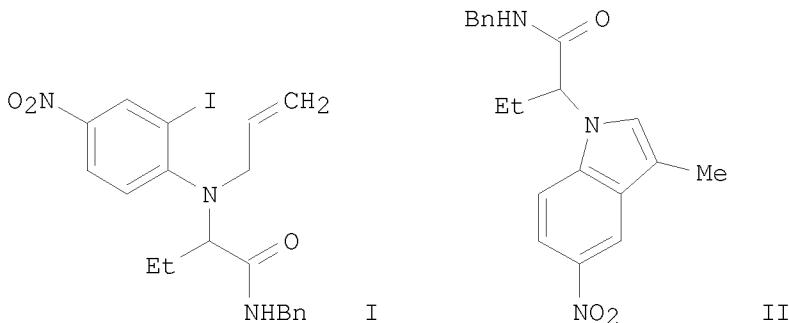
CN Butanoic acid, 2-[[5-[[1S]-1-(aminocarbonyl)-2-methylpropyl]amino]-2,4-dinitrophenyl]amino]-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)  
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2008:837528 HCPLUS  
DOCUMENT NUMBER: 149:200740  
TITLE: New MCR-Heck-Isomerization Cascade toward Indoles  
AUTHOR(S): El Kaim, Laurent; GIZZI, Marion; Grimaud, Laurence  
CORPORATE SOURCE: Laboratoire Chimie et Procedes, Ecole Nationale Supérieure de Techniques Avancées, Paris, 75739, Fr.  
SOURCE: Organic Letters (2008), 10(16), 3417-3419  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 149:200740  
GI



AB The use of ortho-iodonitrophenol in Ugi-Smiles reaction to afford adducts

Updated Search

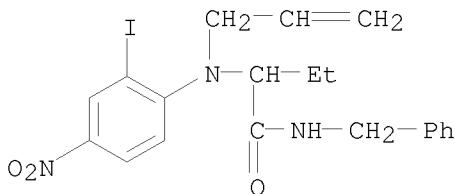
such as I, coupled with Heck cyclization gives new access to indole scaffolds, e.g., II. The sequence can be performed in a one-pot reaction if the residual isocyanide is neutralized prior to the addition of the palladium catalyst.

IT 1040741-64-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [allyl(iodoaryl)amino]amides via Ugi-Smiles coupling between aldehydes, allylamines, isocyanides, and aryl or heteroaryl phenols)

RN 1040741-64-7 HCPLUS

CN Butanamide, 2-[(2-iodo-4-nitrophenyl)-2-propen-1-ylamino]-N-(phenylmethyl)-  
(CA INDEX NAME)

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:621675 HCPLUS

DOCUMENT NUMBER: 150:283353

TITLE: Indirect TLC resolution of amino acid enantiomers after derivatization with Marfey's reagent and its chiral variants

AUTHOR(S): Bhushan, Ravi; Bruckner, Hans; Kumar, Virender; Gupta, Deepak

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, 247 667, India

SOURCE: Journal of Planar Chromatography--Modern TLC (2007), 20(3), 165-171  
CODEN: JPCTE5; ISSN: 0933-4173

PUBLISHER: Akademiai Kiado

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 150:283353

AB A simple and rapid method has been established for indirect separation of the optical isomers of seventeen DL-amino acids by reversed-phase and normal-phase TLC. Amino acids derivatized with 1-fluoro-2,4-dinitrophenyl-5-L-alaninamide (FDNP-L-Ala-NH<sub>2</sub>), 1-fluoro-2,4-dinitrophenyl-5-L-phenylalaninamide (FDNP-L-Phe-NH<sub>2</sub>), or 1-fluoro-2,4-dinitrophenyl-5-L-valinamide (FDNP-L-Val-NH<sub>2</sub>) were spotted on precoated plates. Diastereomers of all the DL amino acids were separated most effectively by normal-phase TLC with phenol-water, 3:1 (v/v), as mobile phase. In reversed-phase TLC, the diastereomers were separated most effectively by use of mobile phases containing acetonitrile and triethylamine-phosphate buffer (50 mM, pH 5.5). The results obtained by

use of the classical Marfey's reagent (FDNP-L-Ala-NH<sub>2</sub>) were compared with those obtained by use of FDNP-L-Phe-NH<sub>2</sub> and FDNP-L-Val-NH<sub>2</sub>. The effects of buffer concentration, pH, and concentration of organic modifier were studied. This

indirect method enabled resolution of DL-amino acids at nanomolar concns.

IT 194736-16-8P

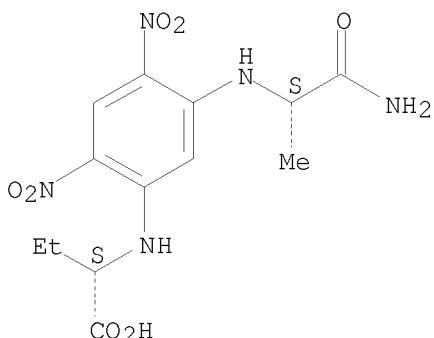
RL: ANT (Analyte); PUR (Purification or recovery); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(preparation of Marfey's reagent-derivatized amino acid diastereomers and their separation via thin layer chromatog.)

RN 194736-16-8 HCPLUS

CN Butanoic acid, 2-[[5-[(1S)-2-amino-1-methyl-2-oxoethyl]amino]-2,4-dinitrophenyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
(8 CITINGS)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:207093 HCPLUS

DOCUMENT NUMBER: 148:462473

TITLE: Virtual screening approaches for the identification of non-lipid autotaxin inhibitors

AUTHOR(S): Parrill, Abby L.; Echols, Uniqua; Nguyen, Tran; Pham, Truc-Chi T.; Hoeglund, Adrienne; Baker, Daniel L.

CORPORATE SOURCE: Department of Chemistry, The University of Memphis, Memphis, TN, 38152, USA

SOURCE: Bioorganic & Medicinal Chemistry (2008), 16(4), 1784-1795

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Autotaxin (ATX, NPP-2) catalyzes the conversion of lysophosphatidyl choline (LPC) to lysophosphatidic acid (LPA), a mitogenic cell survival factor that stimulates cell motility. The high expression of both ATX and receptors for LPA in numerous tumor cell types has produced substantial interest in exploring ATX as an anticancer chemotherapeutic target. ATX inhibitors reported to date are analogs of LPA, a phospholipid, and are

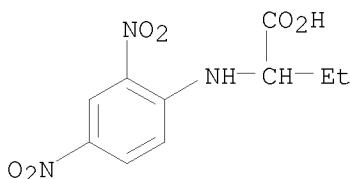
more hydrophobic than is typical of orally bioavailable drugs. This study applied both structure-based and ligand-based virtual screening techniques with hit rates of 20% and 37%, resp., to identify a promising set of nonlipid, drug-like ATX inhibitors. Structure-based virtual screening necessitated development of a homol. model of the ATX catalytic domain due to the lack of structural information on any mammalian NPP family member. This model provided insight into the interactions necessary for ATX inhibition, and produced a suitably diverse training set for the development and application of binary QSAR models for virtual screening. The most efficacious compound identified in this study was able to completely inhibit ATX-catalyzed hydrolysis of 1  $\mu$ M FS-3 (a synthetic, fluorescent LPC analog) at a 10  $\mu$ M concentration

IT 31356-29-3

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(virtual screening approaches for identification of non-lipid autotaxin inhibitors)

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2007:450428 HCAPLUS  
DOCUMENT NUMBER: 147:95385  
TITLE: Smiles Rearrangements in Ugi- and Passerini-Type Couplings: New Multicomponent Access to O- and N-Arylamides  
AUTHOR(S): El Kaiem, Laurent; Gizolme, Marie; Grimaud, Laurence; Oble, Julie  
CORPORATE SOURCE: Laboratoire Chimie et procedes UMR 7652, Ecole Nationale Superieure de Techniques Avancees, Paris, 75015, Fr.  
SOURCE: Journal of Organic Chemistry (2007), 72(11), 4169-4180  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 147:95385  
AB The use of Smiles rearrangement in Ugi- and Passerini-type couplings with electron-deficient phenols allowed very straightforward multicomponent formation of O-aryl- and N-arylamides. Best yields were observed with the highly activated o- and p-nitrophenols, salicylic derivs. giving adducts in lower yields. The scope of these new reactions was further increased

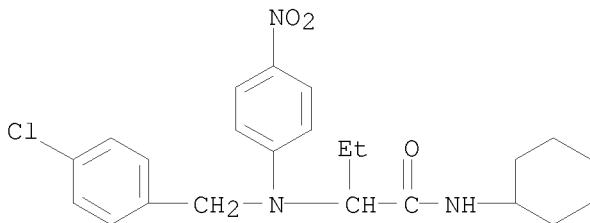
by the successful couplings of heterocyclic phenols such as hydroxypyridines and hydroxypyrimidines.

IT 876013-60-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of O- and N-arylamides via Smiles rearrangements in multicomponent Ugi- and Passerini-type couplings of phenols with carbonyl compds., amines and isocyanides)

RN 876013-60-4 HCPLUS

CN Butanamide, 2-[[[(4-chlorophenyl)methyl](4-nitrophenyl)amino]-N-cyclohexyl-  
(CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:420235 HCPLUS

DOCUMENT NUMBER: 147:72710

TITLE: Novel Series of Potent, Nonsteroidal, Selective Androgen Receptor Modulators Based on 7H-[1,4]oxazino[3,2-g]quinolin-7-ones

AUTHOR(S): Higuchi, Robert I.; Arienti, Kristen L.; Lopez, Francisco J.; Mani, Neelakanda S.; Mais, Dale E.; Caferro, Thomas R.; Long, Yun Oliver; Jones, Todd K.; Edwards, James P.; Zhi, Lin; Schrader, William T.; Negro-Vilar, Andres; Marschke, Keith B.

CORPORATE SOURCE: Discovery Research, Ligand Pharmaceuticals, Inc., San Diego, CA, 92121, USA

SOURCE: Journal of Medicinal Chemistry (2007), 50(10), 2486-2496

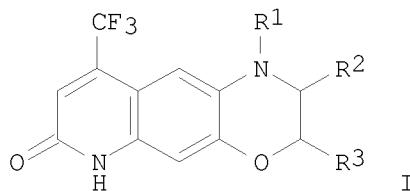
PUBLISHER: CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: American Chemical Society

LANGUAGE: Journal

OTHER SOURCE(S): English

GI: CASREACT 147:72710



AB Recent interest in orally available androgens has fueled the search for new androgens for use in hormone replacement therapy and as anabolic agents. In pursuit of this, a series of novel androgen receptor modulators, 7H-[1,4]oxazino[3,2-g]quinolin-7-ones I (R1 = H, Me, Et, Me2CH, F3CCH2, cyclopropylmethyl, PhCH2, etc.; R2 = H, Me, Et, Me2CH, Me2CHCH2; R3 = H, Me, Et), were synthesized and evaluated in competitive binding assays and an androgen receptor transcriptional activation assay. A number of compds. from the series demonstrated single-digit nanomolar agonist activity in vitro. In addition, lead compound (R)-I (R1 = F3CCH2; R2 = Me; R3 = H) was orally active in established rodent models that measure androgenic and anabolic properties of these agents. In this assay, this compound demonstrated full efficacy in muscle and only partially stimulated the prostate at 100 mg/kg. These data suggest that these compds. may be utilized as selective androgen receptor modulators or SARMs.

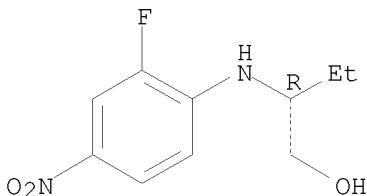
IT 329229-75-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of 7H-[1,4]oxazino[3,2-g]quinolin-7-ones as nonsteroidal selective androgen receptor modulators)

RN 329229-75-6 HCPLUS

CN 1-Butanol, 2-[(2-fluoro-4-nitrophenyl)amino]-, (2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)  
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2007:78981 HCPLUS  
DOCUMENT NUMBER: 147:202511  
TITLE: Capillary zone electrophoresis resolutions of 2,4-dinitrophenyl labeled amino acids enantiomers by N-methylated amino- $\beta$ -cyclodextrins  
AUTHOR(S): Mikus, Peter; Kaniansky, Dusan  
CORPORATE SOURCE: Department of Pharmaceutical Analysis and Nuclear

Pharmacy, Faculty of Pharmacy, Comenius University,  
Bratislava, Slovakia

SOURCE: Analytical Letters (2007), 40(2), 335-347  
CODEN: ANALBP; ISSN: 0003-2719

PUBLISHER: Taylor & Francis, Inc.  
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Capillary zone electrophoresis resolns. of 2,4-dinitrophenyl labeled amino acids (DNP-AAs) enantiomers using three N-methylated amino- $\beta$ -cyclodextrins (CDs) [6I-deoxy-6I-monomethylamino- $\beta$ -CD (M-A- $\beta$ CD), 6I-deoxy-6I-dimethylamino- $\beta$ -CD (diM-A- $\beta$ CD), 6I-deoxy-6I-trimethylammonium- $\beta$ -cyclodextrin (triM-A- $\beta$ CD)] as chiral selectors were studied. These cationogenic selectors, differing in ionization and steric properties, exhibited clear differences in their enantioselectivities. The differences in enantioresoln. observed under identical acid-base conditions (pH 5.2), providing comparable effective charges/mobilities of the CDs, e.g., excellent sepn. of single enantiomeric couples (triM-A- $\beta$ CD, M-A- $\beta$ CD), multicomponent mixts. of enantiomers (M-A- $\beta$ CD), and mixts. of positional isomers (M-A- $\beta$ CD, diM-A- $\beta$ CD), indicated the importance of structural parameters (different degrees of methylation) of the studied chiral selectors in the separation mechanism. The differences in enantioresoln. observed

under various acid base conditions (pH 5.2 and 9.6), providing significant differences of effective charges/mobilities of CDs, e.g., a dramatic decrease in enantioresoln. as well as achiral resolution with uncharged M-A- $\beta$ CD and preserved resolution with permanently charged triM-A- $\beta$ CD, indicated the importance of charge of the studied chiral selectors in the separation mechanism. The present study clearly showed that the studied CD derivs. have great potential as chiral selectors in capillary zone electrophoresis sepn. of DNP-AAs and that their effective use is related to the character of the analyte (structure, hydrophobicity) as well as to working conditions (pH).

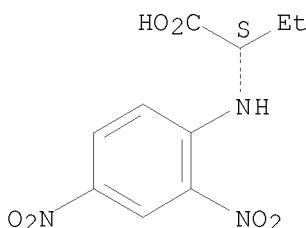
IT 4470-69-3, 2,4-Dinitrophenyl-L- $\alpha$ -amino-n-butyric acid

RL: ANT (Analyte); ANST (Analytical study)  
(analyte; capillary zone electrophoresis resolns. of dinitrophenyl labeled amino acids enantiomers by N-methylated amino- $\beta$ -cyclodextrins)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

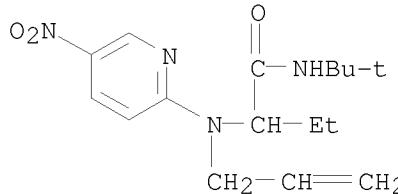


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
(4 CITINGS)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2006:759295 HCPLUS  
 DOCUMENT NUMBER: 145:356744  
 TITLE: Direct Access to Heterocyclic Scaffolds by New  
       Multicomponent Ugi-Smiles Couplings  
 AUTHOR(S): El Kaim, Laurent; Gizolme, Marie; Grimaud, Laurence;  
       Oble, Julie  
 CORPORATE SOURCE: Laboratoire Chimie et Procedes, Ecole Nationale  
       Superieure de Techniques Avancees, Paris, 75739, Fr.  
 SOURCE: Organic Letters (2006), 8(18), 4019-4021  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 145:356744  
 AB New heterocyclic scaffolds can be easily prepared by the coupling of  
       heteroarom. phenols (pyridines, pyrimidines) with carbonyl compds.,  
       amines, and isocyanides. This transformation related to the Ugi reaction  
       probably involves a Smiles rearrangement. The scope of this methodol. is  
       further extended by the successful use of heterocyclic thiols to form  
       highly functionalized thioamides.  
 IT 910311-46-5P  
       RL: SPN (Synthetic preparation); PREP (Preparation)  
       (direct access to heterocyclic scaffolds by multicomponent Ugi-Smiles  
       couplings)  
 RN 910311-46-5 HCPLUS  
 CN Butanamide, N-(1,1-dimethylethyl)-2-[(5-nitro-2-pyridinyl)-2-propen-1-  
       ylamino]- (CA INDEX NAME)



OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS  
 RECORD (21 CITINGS)  
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2006:383697 HCPLUS  
 DOCUMENT NUMBER: 144:432552  
 TITLE: Preparation of substituted anilines as selective  
       androgen receptor modulators  
 INVENTOR(S): Turnbull, Philip Stewart; Larkin, Andrew Lamont;  
       Kaldor, Istvan; Cadilla, Rodolfo; Cowan, David John;  
       Stewart, Eugene Lee  
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA  
 SOURCE: PCT Int. Appl., 134 pp.

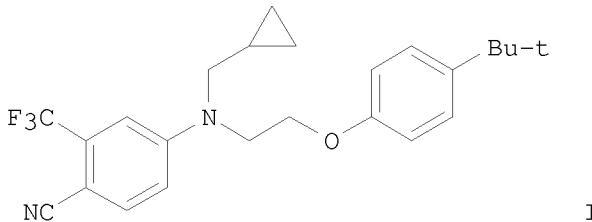
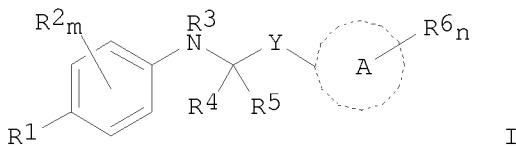
CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044707	A1	20060427	WO 2005-US37094	20051013
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1809275	A1	20070725	EP 2005-812180	20051013
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
JP 2008515998	T	20080515	JP 2007-536962	20051013
US 20080255124	A1	20081016	US 2008-576965	20080312
PRIORITY APPLN. INFO.:			US 2004-618480P	P 20041013
			WO 2005-US37094	W 20051013

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 144:432552; MARPAT 144:432552

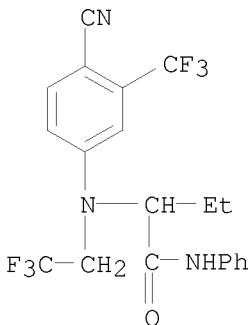
GI



AB This invention relates to non-steroidal compds. I [R1 = CN or NO<sub>2</sub>; R2 = independently CN, NO<sub>2</sub>, halo, etc.; R3 = H, (cyclo)alkyl, alkoxy carbonylalkyl, etc.; R4, R5 = independently H, (cyclo)alkyl, halo, etc., or R4R5 = (un)substituted (hetero)cyclyl; Y = (un)substituted

methylene(oxy), methylenethio, carbonylamino, etc.; A = (hetero)aryl or heterocyclyl; m = 0-2; n = 0-5; R6 = independently (halo)alkyl, halo, hydroxy, etc.] which are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. For example, II was provided in a multi-step synthesis starting from the reaction of 4-fluoro-2-(trifluoromethyl)benzonitrile with 1-cyclopropylmethanamine. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given).

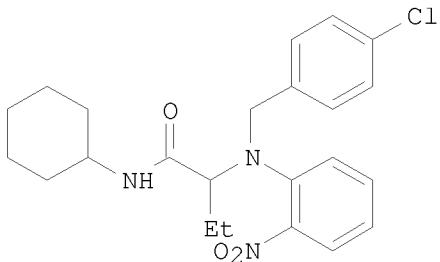
IT 884854-99-3P, 2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-phenylbutanamide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of substituted aniline derivs. as selective androgen receptor modulators)  
 RN 884854-99-3 HCPLUS  
 CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)  
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2005:1345737 HCPLUS  
 DOCUMENT NUMBER: 144:212475  
 TITLE: Phenol Ugi-Smiles systems: strategies for the multicomponent N-arylation of primary amines with isocyanides, aldehydes, and phenols  
 AUTHOR(S): El Kaim, Laurent; Grimaud, Laurence; Oble, Julie  
 CORPORATE SOURCE: Laboratoire de Chimie Organique, UMR CNRS 7652, Ecole Nationale Superieure des Techniques Avancees, Paris, 75015, Fr.  
 SOURCE: Angewandte Chemie, International Edition (2005), 44(48), 7961-7964  
 CODEN: ACIEF5; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal

LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:212475  
 GI

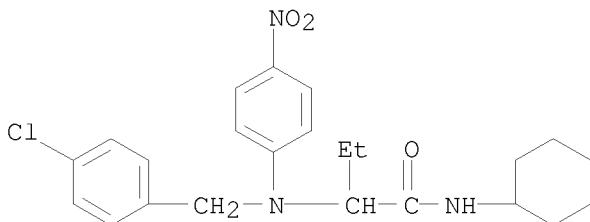


AB A Smiles rearrangement is the key step in the efficient coupling of primary amines with isocyanides, carbonyl compds., and electron-deficient substituted phenols to form N-aryl amines. E.g., reaction of EtCHO, 4-ClC6H4CH2NH2, cyclohexyl isocyanide, and 2-O2NC6H4OH gave 74% aryl amine I. The presence of a nitro or ester group on the resulting adduct allows applications in heterocyclic synthesis.

IT 876013-60-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (multicomponent N-arylation of primary amines with isocyanides, carbonyl compds., and phenols)

RN 876013-60-4 HCAPLUS

CN Butanamide, 2-[(4-chlorophenyl)methyl](4-nitrophenyl)amino]-N-cyclohexyl- (CA INDEX NAME)



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2005:1042201 HCAPLUS  
 DOCUMENT NUMBER: 143:326203  
 TITLE: Arylamines as androgen receptor modulators, their preparation, pharmaceutical compositions, and use in therapy  
 INVENTOR(S): Zhi, Lin; Higuchi, Robert I.; Kallel, E. Adam; Van Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Ruppar, Daniel A.; Pedram, Bijan; Lau, Thomas Lot Stevens;

PATENT ASSIGNEE(S): Miller, Todd  
 SOURCE: Ligand Pharmaceuticals Incorporated, USA  
 PCT Int. Appl., 156 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090282	A1	20050929	WO 2005-US7867	20050311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070254875	A1	20071101	US 2007-590119	20070611
PRIORITY APPLN. INFO.:			US 2004-552690P	P 20040312
			WO 2005-US7867	W 20050311

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 143:326203; MARPAT 143:326203

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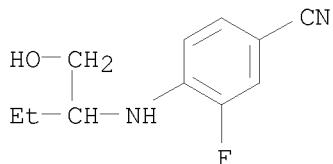
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a group of amines, e.g., I, which act as modulators of androgen receptors and/or androgen receptor binding agents. In compds. I, R1 and R2 are independently selected from H, F, Cl, Br, I, OH, (un)substituted C1-4 alkoxy, etc.; R3, R4, and R5 are independently selected from H, F, Cl, OH, (un)substituted C1-4 alkoxy, (un)substituted C1-4 alkyl, and (un)substituted C1-4 haloalkyl; R6 and R7 are independently selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, (un)substituted C2-6 alkynyl, and (un)substituted C2-6 alkenyl, or R6 and R7 together form a carbonyl; R9 is selected from H, (un)substituted C1-8 alkyl, (un)substituted C2-8 alkenyl, (un)substituted C1-8 haloalkyl, (un)substituted aryl, (un)substituted heteroaryl, etc.; R10 is selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, (un)substituted C2-6 alkynyl, and (un)substituted C2-6 alkenyl; R12 and R13 are independently selected from H, F, Cl, OH, (un)substituted C1-4 alkoxy, (un)substituted amino, (un)substituted C1-6 alkyl, etc.; Z is O, S, (un)substituted C, or (un)substituted N; and n is 0-2; provided that if R1 is NO<sub>2</sub> and R3 is F, then Z is not O; including pharmaceutically acceptable salts, esters, amides or prodrugs thereof. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. containing compds. of the

invention along with a pharmaceutically acceptable carrier, as well as to the use of the compns. for treating various conditions.

3-(Trifluoromethyl)-4-nitrobromobenzene underwent palladium-mediated coupling with chiral pyrrolidinone II followed by reduction to the corresponding pyrrolidine, and desilylation to give alc. III. Oxidation of III to the corresponding aldehyde was followed by addition of TMSCF3 to give IV along with its separable (R,R)-diastereomer. Some of the compds. of the invention act as androgen receptor agonists, others as androgen receptor antagonists, androgen receptor partial agonists, or tissue-specific modulators (no data).

IT 865316-59-2P, 3-Fluoro-4-[(1-hydroxymethylpropyl)amino]benzonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of arylamines as androgen receptor modulators)  
 RN 865316-59-2 HCPLUS  
 CN Benzonitrile, 3-fluoro-4-[(1-(hydroxymethyl)propyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)  
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2005:1004698 HCPLUS  
 DOCUMENT NUMBER: 143:286689  
 TITLE: Preparation of aniline amino acid derivatives as selective androgen receptor modulators  
 INVENTOR(S): Turnbull, Phillip Stewart; Cadilla, Rodolfo; Cowan, David John; Larkin, Andrew Lamont; Kaldor, Istvan; Stewart, Eugene Lee  
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA  
 SOURCE: PCT Int. Appl., 120 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085185	A1	20050915	WO 2005-US7245	20050303
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,				

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,  
 SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,  
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
 MR, NE, SN, TD, TG  
 EP 1725522 A1 20061129 EP 2005-730067 20050303  
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV  
 JP 2007526336 T 20070913 JP 2007-502061 20050303  
 US 20070191479 A1 20070816 US 2006-598508 20060901  
 US 7514470 B2 20090407  
 US 20090163588 A1 20090625 US 2009-392687 20090225  
 US 7723385 B2 20100525  
 PRIORITY APPLN. INFO.: US 2004-549794P P 20040303  
 WO 2005-US7245 W 20050303  
 US 2006-598508 A1 20060901

## ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

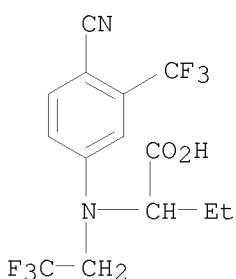
OTHER SOURCE(S): CASREACT 143:286689; MARPAT 143:286689

AB The invention relates to non-steroidal compds. 3,4-R4R3C6H3NR1R2 [R1 is -(Q1)-0-1-R5, where Q1 is alkylene and R5 is H, alkyl, alkenyl, alkynyl, haloalkyl or cycloalkyl; R2 is -Q3-Q4-R6 or -Q3-CN, where Q3 is alkylene, Q4 is CO, CS, C:NR7, R7 is H or alkyl; R6 is alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryloxy or an amino group; R3 is CN, NO2 or halo; R4 is CN, NO2, halo, haloalkyl, alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryl or aryloxy] and their salts, solvates and physiol. functional derivs., that are modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, as well as methods for their synthesis and use. Thus, N2-[4-cyano-3-(trifluoromethyl)phenyl]-N2-(cyclopropylmethyl)-N1-methylglycinamide was prepared from 4-fluoro-2-(trifluoromethyl)benzonitrile by reaction with cyclopropylmethylamine and tert-Bu bromoacetate, followed by ester cleavage and methylamidation.

IT 864283-71-6P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of aniline amino acid derivs. as selective androgen receptor modulators)

RN 864283-71-6 HCPLUS

CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)



STN Search

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
(6 CITINGS)  
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 15 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2003:511102 HCAPLUS  
DOCUMENT NUMBER: 139:73719  
TITLE: Oxidative hair dyes containing N-alkyl derivatives of  
p-benzene diamine as developers  
INVENTOR(S): Knuebel, Georg; Hoeffkes, Horst; Meinigke, Bernd;  
Rose, David; Giesa, Helmut  
PATENT ASSIGNEE(S): Henkel Kommanditgesellschaft Auf Aktien, Germany  
SOURCE: PCT Int. Appl., 49 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

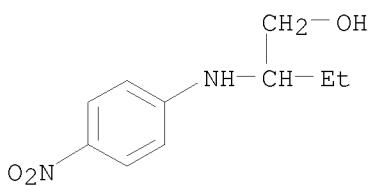
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053370	A2	20030703	WO 2002-EP14292	20021216
WO 2003053370	A3	20031127		
W: JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR				
DE 10163251	A1	20030703	DE 2001-10163251	20011221
EP 1455741	A2	20040915	EP 2002-793025	20021216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRIORITY APPLN. INFO.:			DE 2001-10163251	A 20011221
			WO 2002-EP14292	W 20021216

OTHER SOURCE(S): MARPAT 139:73719

AB The invention relates to means for coloring keratin fibers, in particular human hair, comprising at least one N-alkyl derivative of p-phenylenediamine in a cosmetically-acceptable vehicle, where alkyl = a linear or branched, chiral or achiral C4 - C14 hydroxyalkyl group. The invention further relates to the use of the derivs. for the coloring of keratin fibers and a corresponding method. Thus N-(5-hydroxypentyl)-p-phenylene diamine dihydrochloride was synthesized by reacting 5-amino-1-pentanol and 1-fluoro-4-nitrobenzene in DMSO and triethylamine, followed by catalytic reduction. The product was used as a developer with resorcin as coupler to result a dust gray color.

IT 220159-25-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(oxidative hair dyes containing N-alkyl derivs. of p-benzene diamine as developers)  
RN 220159-25-1 HCAPLUS  
CN 1-Butanol, 2-[(4-nitrophenyl)amino]- (CA INDEX NAME)

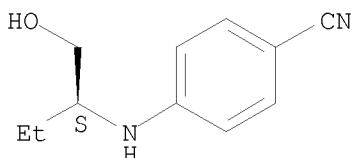
STN Search



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD  
(9 CITINGS)  
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 16 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2003:397213 HCPLUS  
DOCUMENT NUMBER: 139:149559  
TITLE: Palladium-Catalyzed Synthesis of N-Aryloxazolidinones from Aryl Chlorides  
AUTHOR(S): Ghosh, Arun; Sieser, Janice E.; Riou, Maxime; Cai, Weiling; Rivera-Ruiz, Luis  
CORPORATE SOURCE: Process Research and Development, Pfizer Global Research and Development, Groton, CT, 06340-8013, USA  
SOURCE: Organic Letters (2003), 5(13), 2207-2210  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:149559  
AB An efficient method for intermol. N-arylation of oxazolidinones using Pd2dba3 and various phosphine ligands in the presence of a weak base is reported. The conditions allow the use of cheaper aryl chlorides containing functionalities such as enolizable ketones, amides, etc., which would be incompatible with other coupling methods. The coupling reaction can be used to prepare enantiopure N-aryl  $\beta$ -amino alcs. Depending on the stereoelectronic nature of the aryl chloride, careful choice of ligand was necessary for the success of these reactions.  
IT 572923-29-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed synthesis of N-aryloxazolidinones from aryl chlorides and hydrolysis to arylamino alcs.)  
RN 572923-29-6 HCPLUS  
CN Benzonitrile, 4-[(1S)-1-(hydroxymethyl)propyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 35 THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (35 CITINGS)  
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS

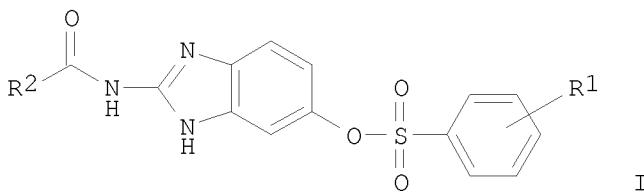
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 17 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2003:259734 HCAPLUS  
 DOCUMENT NUMBER: 138:271683  
 TITLE: Preparation of  
 2-(acylamino)-5-(benzenesulfonyloxy)benzimidazole  
 compounds and their use for the treatment of cancer  
 Inventor(s): Clerc, Francois; Hamy, Francois; Depaty, Isabelle;  
 Angoullant-Boniface, Odile; Roesner, Manfred  
 Patent Assignee(s): Aventis Pharma S.A., Fr.  
 Source: Eur. Pat. Appl., 31 pp.  
 CODEN: EPXXDW  
 Document Type: Patent  
 Language: English  
 Family Acc. Num. Count: 1  
 Patent Information:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1298125	A1	20030402	EP 2001-402460	20010926
R: AT, BE, CH, IE, SI, LT,	DE, DK, ES, FR, LV, FI, RO, MK,	GB, GR, IT, LI, LU, NL, SE, MC, PT, CY, AL, TR		
CA 2461622	A1	20030410	CA 2002-2461622	20020926
CA 2461622	C	20081202		
WO 2003028721	A2	20030410	WO 2002-EP11353	20020926
WO 2003028721	A3	20031211		
W: AE, AG, AL, AM, AT, AU, AZ, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002337151	A1	20030414	AU 2002-337151	20020926
AU 2002337151	B2	20070426		
EP 1432417	A2	20040630	EP 2002-772370	20020926
EP 1432417	B1	20080220		
R: AT, BE, CH, IE, SI, LT,	DE, DK, ES, FR, LV, FI, RO, MK,	GB, GR, IT, LI, LU, NL, SE, MC, PT, CY, AL, TR, BG, CZ, EE, SK		
BR 2002012856	A	20040914	BR 2002-12856	20020926
CN 1558761	A	20041229	CN 2002-818745	20020926
CN 100346786	C	20071107		
HU 2004001756	A2	20050128	HU 2004-1756	20020926
HU 2004001756	A3	20050628		
JP 2005504112	T	20050210	JP 2003-532053	20020926
JP 4510450	B2	20100721		
NZ 531246	A	20060630	NZ 2002-531246	20020926
AT 386517	T	20080315	AT 2002-772370	20020926
PT 1432417	E	20080523	PT 2002-772370	20020926
ES 2301682	T3	20080701	ES 2002-772370	20020926
MX 2004002042	A	20040607	MX 2004-2042	20040303
ZA 2004001887	A	20050531	ZA 2004-1887	20040308

NO 2004001214	A 20040624	NO 2004-1214	20040323
NO 327008	B1 20090406		
IN 2004CN00600	A 20060113	IN 2004-CN600	20040323
IN 227958	A1 20090306		
US 20050014811	A1 20050120	US 2004-808889	20040325
US 7041668	B2 20060509		
HR 2004000293	A2 20050630	HR 2004-293	20040325
KR 891439	B1 20090403	KR 2004-704365	20040325
HK 1068551	A1 20080201	HK 2005-101028	20050207
PRIORITY APPLN. INFO.:		EP 2001-402460	A 20010926
		WO 2002-EP11353	W 20020926

OTHER SOURCE(S): MARPAT 138:271683  
GI



AB New benzimidazole compds. of formula (I) [wherein R1 = 4-NH2, 4-alkylamino or cycloalkylamino eventually substituted with an acyl or its derivative, hydroxy, amino, alkoxy, heterocyclyl, or aryl group; R2 = (1) alkyl eventually substituted by amino, acid, acid derivative, alkoxy, aryl or OH groups, (2) arylalkyl eventually substituted by alkoxy, halogeno, amino, acid or acid derivs., (3) alkoxy eventually substituted by aryl, (4) amino, NHR3, or NR3R4 (wherein R3, R4 = H, alkyl, alkylaryl, aryl or together form an alkylene chain)] or pharmaceutically acceptable salts thereof, which are useful for treating cancer diseases, are prepared. These compds. I are inhibitors of cyclin-dependent kinases (CKDs, in particular CDK4) which are regulators for progression of the cell cycle at cell cycle checkpoints, and are effective in inhibiting the proliferation of neoplastic cells. Thus, 15.6 g 2-amino-5-(4-fluorophenylsulfonyloxy)nitrobenzene were combined with 25 mL ethanolamine in 100 mL ethylene glycol in a round bottom flask and heated to reflux for 90 min to give, after workup, 15.5 g 2-amino-5-[4-(2-hydroxyethyl)aminophenylsulfonyloxy]nitrobenzene (II). II (15.5 g) in 75 mL MeOH and 75 mL DMF were hydrogenated under atmospheric pressure

with a catalytic amount of Raney Nickel, filtered to remove the catalyst followed by washing the catalyst with MeOH. The filtrate and the washing were combined, concentrated under reduced pressure, taken up in 150 mL MeOH and 30 mL glacial acetic acid, treated with 10.3 g 1,3-bis(methoxycarbonyl)-2-methyl-2-thiopseudourea, and heated to reflux with stirring for 3 h to give, after crystallization from methanol, 7.4 g Me 5-[4-(2-hydroxyethyl)aminophenylsulfonyloxy]benzimidazole-2-carbamate (III). III and Me 5-(4-aminophenylsulfonyloxy)benzimidazole-2-carbamate showed IC50 of 1.43 and 0.28  $\mu$ M, resp., against CDK4/CyclinD1 kinase.

IT 503545-69-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

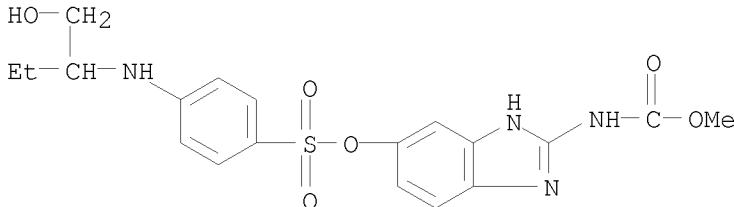
## STN Search

## (Uses)

(preparation of 2-(acylamino)-5-(benzenesulfonyloxy)benzimidazole compds. as inhibitors of cyclin-dependent kinases for treatment of cancer)

RN 503545-69-5 HCPLUS

CN Benzenesulfonic acid, 4-[[1-(hydroxymethyl)propyl]amino]-, 2-[(methoxycarbonyl)amino]-1H-benzimidazol-6-yl ester (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 18 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:676021 HCPLUS

DOCUMENT NUMBER: 137:201318

TITLE: Preparation of tricyclic quinolinone androgen receptor modulator compounds

INVENTOR(S): Higuchi, Robert I.; Zhi, Lin; Karanewsky, Donald S.; Thompson, Anthony W.; Caferro, Thomas R.; Mani, Neelakandha S.; Chen, Jyun-Hung; Cummings, Marquis L.; Edwards, James P.; Adams, Mark E.; Deckhut, Charlotte L. F.

PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 142 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068427	A1	20020906	WO 2002-IB538	20020223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20020183314	A1	20021205	US 2002-80503	20020222
US 7214690	B2	20070508		
CA 2434727	A1	20020906	CA 2002-2434727	20020223

AU 2002236115	A1	20020912	AU 2002-236115	20020223
EP 1368357	A1	20031210	EP 2002-702590	20020223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002007543	A	20040427	BR 2002-7543	20020223
CN 1492872	A	20040428	CN 2002-805529	20020223
JP 2004524317	T	20040812	JP 2002-567937	20020223
IN 2003DN01286	A	20050527	IN 2003-DN1286	20030813
IN 233059	A1	20090403		
MX 2003007422	A	20031204	MX 2003-7422	20030819
US 20070072849	A1	20070329	US 2006-601251	20061117
US 20080300241	A9	20081204		

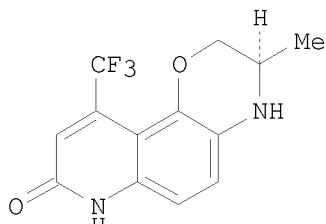
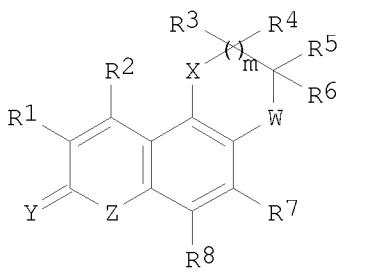
PRIORITY APPLN. INFO.:

US 2001-271115P	P	20010223
US 2002-80503	A1	20020222
WO 2002-IB538	W	20020223

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 137:201318

GI



AB Title compds. I [R1 = H, F, Cl, Br, I, NO<sub>2</sub>, etc.; R2 = H, F, Cl, Br, I, CF<sub>3</sub>, CF<sub>2</sub>Cl, CF<sub>2</sub>H, etc.; R3-4 = H, alkoxy, SOO-2, amino, alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, arylalkyl, heteroaryl, alkynyl, etc., or R3-4 taken together form a 3-8 membered (un)saturated (hetero)cyclic ring or R3, R5 taken together form a 3-8 membered (un)saturated ring or R3, R6 taken together form a 3-8 membered (un)saturated ring; R5-6 = H, CF<sub>3</sub>, CF<sub>2</sub>Cl, CF<sub>2</sub>H, alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, arylalkyl, heteroaryl, alkynyl, alkenyl, etc.; R7 = H, F, Cl, Br, I, alkyl, haloalkyl, heteroalkyl, aryl, heteroaryl, alkoxy, etc.; R8 = H, F, Cl, Br, I, alkyl, haloalkyl, heteroalkyl, aryl, heteroaryl, alkoxy, etc.; m = 0-2; W = O, SOO-2, N(H, alkyl, etc.,); X, Z = O, SOO-2, NH, etc.; Y = O, S, N(H, alkyl, etc.,), etc.] were prepared. Over 50 synthetic examples were provided. For instance, 5-chloro-1,3-phenylenediamine was reacted with 4,4,4-trifluoroacetacetate in EtOH at reflux for 18 h to give 5-Amino-7-chloro-3,4-dihydro-4-hydroxy-4-(trifluoromethyl)-1H-quinolin-2-one (37%). This was reduced (EtOH, KOAc, 10% Pd/C-H<sub>2</sub>, 2 h) to give 5-Amino-3,4-dihydro-4-hydroxy-4-(trifluoromethyl)-1H-quinolin-2-one (100%). This substrate was then subjected to the following reaction sequence: i. NaNO<sub>2</sub>/H<sub>2</sub>SO<sub>4</sub>; ii. EtOAc, i-PrNH<sub>2</sub>, NBS; iii. DMF, BnBr, CsF; iv. MsOH, HOAc; v. THF, NMM, Ph<sub>3</sub>P, DIAD, (R)-Boc-alinol; vi. CH<sub>2</sub>Cl<sub>2</sub>, TFA; vii. PhMe, Pd(O)Ligand, NaOBu-t; viii. HOAc, HCl, 90°, 4 h to give II. I are agonists, partial agonists and/or antagonists for androgen receptors (AR).

IT 329229-75-6P, (R)-(+)-2-[2-Fluoro-4-nitrophenyl]amino]butanol

STN Search

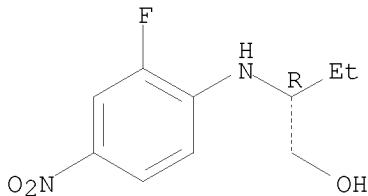
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of tricyclic quinolinone androgen receptor modulator compds.)

RN 329229-75-6 HCPLUS

CN 1-Butanol, 2-[(2-fluoro-4-nitrophenyl)amino]-, (2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 19 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:565601 HCPLUS

DOCUMENT NUMBER: 135:297787

TITLE: Evaluation of novel dendrimer chiral stationary phases using HPLC

AUTHOR(S): Mathews, B. T.; Beezer, A. E.; Snowden, M. J.; Hardy, M. J.; Mitchell, J. C.

CORPORATE SOURCE: Medway Sciences, Natural Resources Institute, University of Greenwich, Chatham, ME4 4TB, UK

SOURCE: Chromatographia (2001), 53(3/4), 147-155

CODEN: CHRGB7; ISSN: 0009-5893

PUBLISHER: Friedrich Vieweg & Sohn Verlagsgesellschaft mbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reversed phase chromatog. properties of the [G1]-L-glutamic acid Et ester-AC-silica (1), [G2]-L-glutamic acid Et ester-AC-silica (2) and the [G1]-L-glutamic acid t-Bu ester-AC-silica (3) dendrimer stationary phases were evaluated. Initial studies involved the comparison between these phases with a classic reversed phase (i.e. ODS1) by the separation of a standard

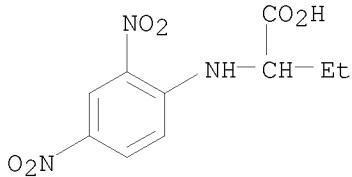
reversed phase test mixture composed of dimethylphthalate, nitrobenzene, anisole, diphenylamine and fluorene. Sepns. were achieved with comparable performance to those obtained with the conventional reversed phase (ODS1). However, the chromatog. selectivity exhibited by the dendrimer stationary phases was different from that of the ODS1 phase. On a per mol basis, the dendrimers exhibited similar (and sometimes greater) affinity for these analytes compared with the ODS1 ligand. Subsequent chromatog. expts. were conducted upon the dendrimer chiral stationary phases using chiral analytes under reversed phase and normal phase conditions. Chiral resolution was not observed

IT 31356-29-3

RL: ARU (Analytical role, unclassified); ANST (Analytical study)

(evaluation of novel dendrimer chiral stationary phases by HPLC separation

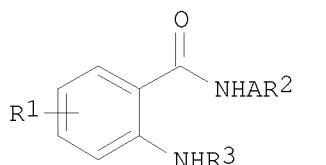
of)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
 (7 CITINGS)  
 REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 20 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2001:319860 HCAPLUS  
 DOCUMENT NUMBER: 134:340354  
 TITLE: Preparation of anthranilamides as inhibitors of cGMP phosphodiesterase.  
 INVENTOR(S): Oku, Teruo; Sawada, Kozo; Kuroda, Akio; Kayakiri, Natsuko; Urano, Yasuharu; Sawada, Yuki; Mizutani, Tsuyoshi  
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan; Oku, Noriko; Oku, Chikako; Oku, Tomohito  
 SOURCE: PCT Int. Appl., 105 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030745	A1	20010503	WO 2000-JP7308	20001019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			AU 1999-3652	A 19991025
OTHER SOURCE(S):		MARPAT 134:340354		
GI				



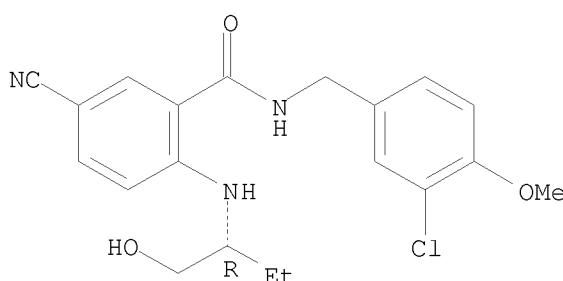
AB Title compds. I; [R1 = NO<sub>2</sub>, amino, cyano, haloalkyl, acyl, halo, etc.; R2 = H, OH, alkoxy, alkyl, cycloalkyl, (substituted) aryl, heterocyclyl; A = alkylene; R3 = (substituted) heterocyclyl, CR<sub>4</sub>R<sub>5</sub>R<sub>6</sub>; R<sub>4</sub>, R<sub>5</sub> (substituted) carbamoyl, alkyl; R<sub>4</sub>R<sub>5</sub>C = = (substituted) carbocyclyl; R<sub>6</sub> = H, alkyl], were prepared. Thus, reaction of 2-(cyclopentylamino)-5-nitrobenzoic acid with BuNH<sub>2</sub> in DMF in the presence of 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide and 1-hydroxybenzotriazole gave N-butyl-2-(cyclopentylamino)-5-nitrobenzamide. The latter inhibited human platelet cGMP phosphodiesterase with IC<sub>50</sub> <10 nM.

IT 337360-80-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of anthranilamides as inhibitors of cGMP phosphodiesterase)

RN 337360-80-2 HCPLUS

CN Benzamide, N-[(3-chloro-4-methoxyphenyl)methyl]-5-cyano-2-[(1R)-1-(hydroxymethyl)propyl]amino- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
 (4 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 21 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:244346 HCPLUS

DOCUMENT NUMBER: 135:55146

TITLE: Separation of multicomponent mixtures of 2,4-dinitrophenyl labelled amino acids and their enantiomers by capillary zone electrophoresis

AUTHOR(S): Mikus, Peter; Kaniansky, Dusan; Fanali, Salvatore

CORPORATE SOURCE: Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava, SK-84215, Slovakia

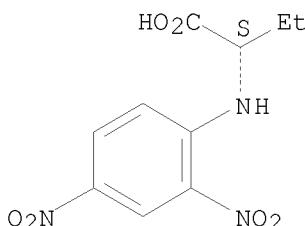
SOURCE: Electrophoresis (2001), 22(3), 470-477  
 CODEN: ELCTDN; ISSN: 0173-0835  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The use of capillary zone electrophoresis (CZE) for the separation of a group of 33 2,4-dinitrophenyl labeled amino acids (DNP-AA), including DNP-AA racemates, DNP-L-AA enantiomers and achiral DNP-AAs, was studied.  $\alpha$ -,  $\beta$ - And  $\gamma$ -cyclodextrins (CDs) and their derivs. (hydroxypropyl derivs. of  $\alpha$ -,  $\beta$ - and  $\gamma$ -CDs, polymeric  $\beta$ -CD and 6A-methylamino- $\beta$ -cyclodextrin (MA- $\beta$ -CD)) served as complexing agents and chiral selectors. Although native  $\alpha$ - and  $\gamma$ -CDs and their derivs. influenced the effective mobilities of the studied DNP-AAs in different ways, they generally failed to resolve enantiomers of the individual DNP-AAs. However,  $\beta$ -CD and all of its derivs. are effective in this respect. Of these, the best results were achieved with a pos. charged MA- $\beta$ -CD and this chiral selector resolved enantiomers of ten DNP-AA racemates available for this study. However, a complete resolution of these enantiomers in one CZE run required that the effect of the chiral selector be complemented by complexing effects of polyvinyl pyrrolidone (PVP) or  $\gamma$ -CD. Complexing and chiral recognition capabilities of MA- $\beta$ -CD combined with complexing effects of  $\gamma$ -CD and PVP provided separating conditions suitable for the CZE seps. of multicomponent mixts. of DNP-AAs with preserved resolns. of the enantiomers. For example, a mixture consisting of 43 DNP-AA constituents was resolved using an MA- $\beta$ -CD/ $\gamma$ -CD combination with three peak overlaps.

IT 4470-69-3, L-DNP- $\alpha$ -amino-n-butyric acid  
 RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)  
 (separation of multicomponent mixts. of 2,4-dinitrophenyl labeled amino acids and their enantiomers by capillary zone electrophoresis)

RN 4470-69-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)  
 REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 22 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2001:167998 HCAPLUS  
 DOCUMENT NUMBER: 134:222717  
 TITLE: Preparation of androgen receptor ligands

## STN Search

INVENTOR(S): Higuchi, Robert; Arienti, Kristen L.; Neelakandha, Mani; Pio, Barbara; Zhi, Lin; Chen, Penghui; Caferro, Thomas R.

PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 173 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

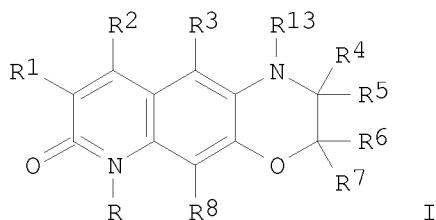
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016139	A1	20010308	WO 2000-US23520	20000825
WO 2001016139	A9	20020919		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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CA 2383077	A1	20010308	CA 2000-2383077	20000825
EP 1212330	A1	20020612	EP 2000-957854	20000825
EP 1212330	B1	20060419		
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BR 2000013597	A	20020716	BR 2000-13597	20000825
US 6462038	B1	20021008	US 2000-648684	20000825
TR 2002000507	T2	20021021	TR 2002-507	20000825
HU 2002002814	A2	20021228	HU 2002-2814	20000825
HU 2002002814	A3	20031128		
JP 2003508402	T	20030304	JP 2001-519705	20000825
AU 778655	B2	20041216	AU 2000-69414	20000825
AT 323709	T	20060515	AT 2000-957854	20000825
ZA 2002001056	A	20030506	ZA 2002-1056	20020206
IN 2002MN00202	A	20051104	IN 2002-MN202	20020215
NO 2002000913	A	20020429	NO 2002-913	20020225
MX 2002002032	A	20030519	MX 2002-2032	20020226
BG 106550	A	20021031	BG 2002-106550	20020325
US 20030186970	A1	20031002	US 2002-238363	20020909
US 20070167445	A1	20070719	US 2006-340282	20060125
PRIORITY APPLN. INFO.:			US 1999-150988P	P 19990827
			US 2000-648684	A3 20000825
			WO 2000-US23520	W 20000825
			US 2002-238363	A1 20020909

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 134:222717

GI



AB Title compds., e.g., I [R = H, alkyl, aryl, etc.; R1 = H, halo, alkyl, (hetero)aryl, etc.; R2 = H, alkyl, alkoxy(methyl), (hetero)aryl, etc.; R4,R5 = H, alkyl, alkoxy, (hetero)aryl, etc.; R6,R7,R13 = H, alkyl, (hetero)aryl, etc.; R8 = H, halo, alkyl, alkoxy, etc.] were prepared. Thus, 2-amino-5-nitrophenol was cyclocondensed with ClCH<sub>2</sub>COCl and the product converted in 3 steps to 7-amino-3,4-dihydro-4-methyl-2H-1,4-benzoxazine which was condensed with CF<sub>3</sub>COCH<sub>2</sub>CO<sub>2</sub>Et and the product treated with PPA to give I (R = R1 = R3-R8 = H, R2 = CF<sub>3</sub>, I<sub>3</sub> = Me). Data for biol. activity of title compds. were given.

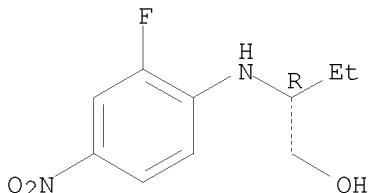
IT 329229-75-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of androgen receptor ligands)

RN 329229-75-6 HCPLUS

CN 1-Butanol, 2-[(2-fluoro-4-nitrophenyl)amino]-, (2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:63979 HCPLUS

DOCUMENT NUMBER: 134:100871

TITLE: Benzimidazolone derivatives, method of preparation and their use as phosphodiesterase inhibitors

INVENTOR(S): Sawada, Kozo; Inoue, Takayuki; Sawada, Yuki; Mizutani, Tsuyoshi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

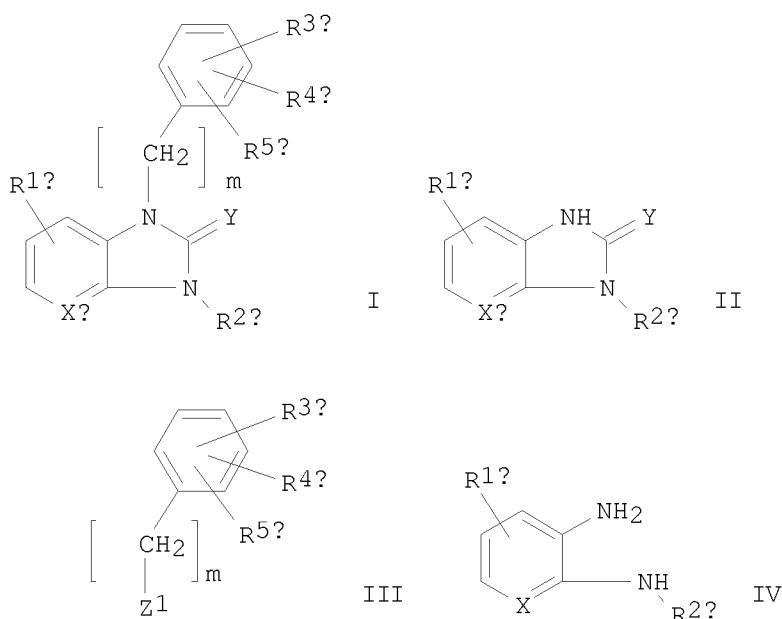
## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005770	A1	20010125	WO 2000-JP4687	20000712
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2379554	A1	20010125	CA 2000-2379554	20000712
AU 2000058531	A	20010205	AU 2000-58531	20000712
EP 1196391	A1	20020417	EP 2000-944421	20000712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 2002000161	T2	20020521	TR 2002-161	20000712
BR 2000013041	A	20020716	BR 2000-13041	20000712
HU 2002002186	A2	20021228	HU 2002-2186	20000712
HU 2002002186	A3	20030228		
JP 2003505376	T	20030212	JP 2001-511431	20000712
ZA 2002000029	A	20030402	ZA 2002-29	20020102
IN 2002KN00019	A	20050311	IN 2002-KN19	20020103
MX 2002000340	A	20020621	MX 2002-340	20020109
US 6582351	B1	20030624	US 2002-30979	20020116
PRIORITY APPLN. INFO.:			AU 1999-1747	A 19990721
			AU 1999-2730	A 19990909
			WO 2000-JP4687	W 20000712

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 134:100871

GI



AB Benzimidazolone derivs. I, its prodrugs or pharmaceutically acceptable salts thereof, a method for their preparation, pharmaceutical compns. containing

them, and usefulness in treatment or prevention of diseases mediated by cyclic guanosine-3',5'-monophosphate phosphodiesterase (cGMP-PDE) are claimed. In I, Xa = CH or N; ya = O, S; R1a = halogen, cyano, NO<sub>2</sub> carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, lower alkyl, halo(lower)alkyl, lower alkoxy, acyl, lower alkanesulfonyl. R2a = lower alkyl, cycloalkyl or heterocyclic group, among which the lower alkyl group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, lower alkylamino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower alkanesulfonyl, lower alkylenedioxy, carbamoyl, lower alkyl carbamoyl and sulfamoyl; and the cycloalkyl group and the heterocyclic group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl. R3a, R4a and R5a = same or different, H, halogen, lower alkanoyl, carboxy, protected carboxy, carbamoyl, nitro, cyano, lower alkyl optionally substituted by hydroxy, lower alkoxy or lower-alkoxy-substituted aralkyl; or two of R3a, R4a and R5a may combine together to form a lower alkylenedioxy. M = 1, 2, provided that when R3a = H, R4a = lower alkoxy and R5a = H, halogen, cyano, lower alkyl, lower alkoxy, protected carboxy, carboxy or nitro, then (1) the lower alkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower

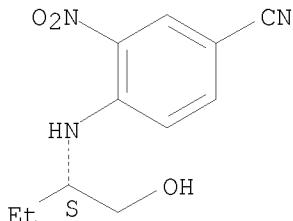
alkanesulfonyl, lower alkylenedioxy, carbamoyl, lower alkyl carbamoyl and sulfamoyl, (2) the cycloalkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl, (3) the heterocyclic group for R2a = pyrrolidinyl, dioxanyl and piperidyl which groups may be substituted with protected carboxy, acyl, lower alkanesulfonyl, carbamoyl or sulfamoyl, (4) R1a = carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, acyl, or lower alkanesulfonyl, (5) Xa = N; (6) m = 2; or (7) yra = S. Pharmaceutical compns. containing the above compds. are claimed (with test data provided for 8 compds.) to be effective for treatment or prevention of diseases mediated by cGMP-PDE: angina, hypertension, pulmonary hypertension, congestive heart failure, glomerular diseases, renal tubulo-intestinal diseases, renal failure, atherosclerosis, conditions of reduced blood vessel patency, peripheral vascular disease, stroke, bronchitis, asthma, allergic rhinitis, urticaria, glaucoma, diseases characterized by disorders of gut motility, erectile dysfunction, female sexual dysfunction, impotence, diabetic complications, micturition disorder, or incontinence and storage of urine disorder. The method of preparation comprises reacting II with III (Z1 = halogen) in the presence of base. III are made by intramol. cyclization of IV (X = N). For example, to a solution of 1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (200 mg) in anhydrous DMF (2 mL) was added portionwise NaH (29.3 mg, 60% dispersion in mineral oil) at 5° under N2 atmosphere, and the mixture was stirred at room temperature for 30 min. After adding 3,4-dimethoxybenzyl bromide (154 mg), the mixture was stirred at room temperature for 2 h. After workup, 3-(3,4-dimethoxybenzyl)-1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (217.9 mg) was obtained as a colorless solid.

IT 320406-03-9P, 4-[(S)-1-Ethyl-2-hydroxyethyl]amino]-3-nitrobenzonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; benzimidazolone derivs., method of preparation and use as phosphodiesterase inhibitors)

RN 320406-03-9 HCAPLUS

CN Benzonitrile, 4-[(1S)-1-(hydroxymethyl)propyl]amino]-3-nitro- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS

REFERENCE COUNT: 13 RECORD (11 CITINGS)  
 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 24 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2000:86260 HCPLUS  
 DOCUMENT NUMBER: 132:293994  
 TITLE: Mass spectrometric fragmentation reactions. XXXIX. The investigation of N-dinitrophenyl derivatives of amino acids by electron/chemical ionization using a particle beam interface

AUTHOR(S): Kaussmann, M.; Budzikiewicz, H.  
 CORPORATE SOURCE: Institut fur Organische Chemie der Universitat zu Keln, Keln, D-50939, Germany

SOURCE: Spectroscopy (Amsterdam) (1999), 14(2), 67-82  
 CODEN: SPIJDZ; ISSN: 0712-4813

PUBLISHER: IOS Press

DOCUMENT TYPE: Journal

LANGUAGE: English

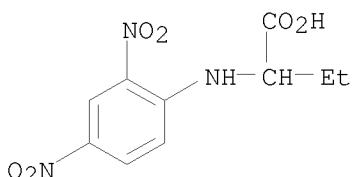
AB The EI and CI mass spectra of 2,4-dinitrophenyl(DNP)-amino acids and oligopeptides give characteristic mass spectra when a particle beam interface is used for introduction. They differ from mass spectra obtained after direct insertion into the ion source. In the particle beam interface the major part of the mols. suffers degradation by contact with metal surfaces such as decarboxylation and reduction of the nitro groups. The final products are benzimidazole derivs. carrying in the 2-position the residue of the resp. amino acid. These products show characteristic fragmentation reactions which allow to identify isomeric amino acids. For DNP-di- and oligopeptides an identification of the N-terminal amino acid is always possible, that of the C-terminus with restrictions.

IT 31356-29-3

RL: PRP (Properties)  
 (investigation of dinitrophenyl derivs. of amino acids by mass spectrometric fragmentation reactions on beam surface)

RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1999:691067 HCPLUS

DOCUMENT NUMBER: 131:310451

TITLE: Preparation of anthranilamides as of cGMP-phosphodiesterase inhibitors

## STN Search

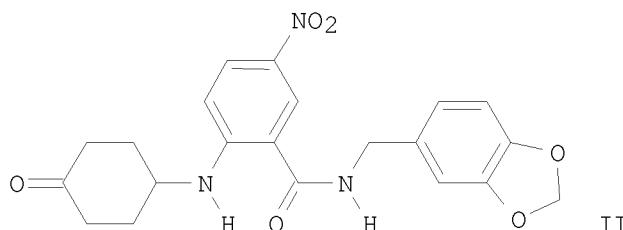
INVENTOR(S): Oku, Teruo; Sawada, Kozo; Kuroda, Akio; Inoue, Takayuki; Kayakiri, Natsuko; Sawada, Yuki; Mizutani, Tsuyoshi  
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 192 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9954284	A1	19991028	WO 1999-JP2028	19990415
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2328413	A1	19991028	CA 1999-2328413	19990415
AU 9931708	A	19991108	AU 1999-31708	19990415
AU 758298	B2	20030320		
BR 9909781	A	20001219	BR 1999-9781	19990415
TR 2000003037	T2	20010122	TR 2000-3037	19990415
EP 1080069	A1	20010307	EP 1999-913686	19990415
EP 1080069	B1	20030319		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001508811	T	20010703	JP 1999-552766	19990415
HU 2001001793	A2	20011028	HU 2001-1793	19990415
HU 2001001793	A3	20030228		
AT 234810	T	20030415	AT 1999-913686	19990415
IN 2000KN00351	A	20050311	IN 2000-KN351	20000925
ZA 2000005243	A	20020114	ZA 2000-5243	20000928
MX 2000009950	A	20010405	MX 2000-9950	20001011
US 6384080	B1	20020507	US 2001-509541	20010423
US 20020193614	A1	20021219	US 2002-50789	20020118
PRIORITY APPLN. INFO.:			AU 1998-3085	A 19980420
			AU 1998-5851	A 19980911
			AU 1998-7781	A 19981218
			WO 1999-JP2028	W 19990415
			US 2001-509541	A1 20010423

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 131:310451

GI



AB R4NHZ1CONHZR3 [I; R3 = H, OH, alkoxy, aryl, etc.; R4 = alkoxy, heterocyclyl, (alkyl)amino, etc.; Z = alkylene; Z1 = e-withdrawing group-substituted (halo)-1,2-phenylene] were prepared. Thus, 2-fluoro-5-nitrobenzoic acid was amidated by 1,3-benzodioxole-5-methylamine and the product aminated by 4-aminocyclohexanol to give, after oxidation, title compound II. Data for biol. activity of I were given.

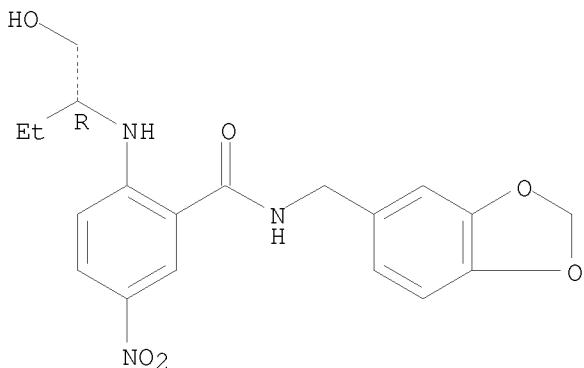
IT 247566-88-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of anthranilamides as of cGMP-phosphodiesterase inhibitors)

RN 247566-88-7 HCPLUS

CN Benzamide, N-(1,3-benzodioxol-5-ylmethyl)-2-[(1R)-1-(hydroxymethyl)propyl]amino]-5-nitro- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(13 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 26 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1999:458983 HCPLUS

DOCUMENT NUMBER: 131:153216

TITLE: Stereochemical resolution of racemates, in HPLC, using a chiral stationary phase based upon immobilized  $\alpha$ -chymotrypsin. Part 1. Structural chiral separations

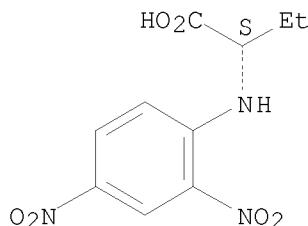
AUTHOR(S): Felix, G.; Descorps, V.  
 CORPORATE SOURCE: ENSCPB, Talence, F-33402, Fr.  
 SOURCE: Chromatographia (1999), 49(11/12), 595-605  
 CODEN: CHRGB7; ISSN: 0009-5893  
 PUBLISHER: Friedrich Vieweg & Sohn Verlagsgesellschaft mbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB  $\alpha$ -Chymotrypsin was immobilized on an epoxide derivatized silica gel by an in-situ immobilization process. Several protected amino acids and other racemates were resolved by a structural recognition mechanism. The immobilization process and the stability of this  $\alpha$ -chymotrypsin stationary phase were studied. Mobile phase parameters including the ionic strength, pH, and the effects of organic modifiers were also investigated. The retention, efficiency, and stereoselectivity of the solutes appear to be related to their mol. structure, hydrophobicity, and electrostatic interactions. These relationships determine the recognition mechanism and the position of each enantiomer in the active site.

IT 4470-69-3P  
 RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical study); PREP (Preparation)  
 (HPLC resolution with chiral stationary phase based upon silica-immobilized chymotrypsin)

RN 4470-69-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 33 THERE ARE 33 CAPLUS RECORDS THAT CITE THIS RECORD (33 CITINGS)  
 REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 27 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1999:188279 HCPLUS  
 DOCUMENT NUMBER: 130:282358  
 TITLE: Solid-phase peptide synthesis by fragment condensation: coupling in swelling volume  
 AUTHOR(S): Rinnova, Marketa; Lebl, Michal; Soucek, Milan  
 CORPORATE SOURCE: Institute of Organic Chemistry and Biochemistry, Prague, CZ-166 10/6, Czech Rep.  
 SOURCE: Letters in Peptide Science (1999), 6(1), 15-22  
 CODEN: LPSCEM; ISSN: 0929-5666  
 PUBLISHER: Kluwer Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The condensation of short peptides to resin-bound fragments was examined

with respect to high coupling yields with only a small molar excess of a peptide in the reaction solution. The best results were achieved by the addition

of reactants (C-unprotected peptide, diisopropylcarbodiimide, and HOBT) dissolved in a so-called swelling volume of an appropriate solvent to a dry resin with an attached N-deprotected peptide chain. Each coupling step was followed by the end-capping of unreacted resin-bound peptide with 2,4-dinitrofluorobenzene. The substituted dinitroaniline chromophore formed in this reaction made the detection and separation of deletion peptides easy. Both conventional and "swelling volume" methods were compared on parallel syntheses of the HIV-1 protease C-terminal 78-99 fragment. The yields of the isolated heptacosapeptide were 21 and 81% in favor of the "swelling volume" procedure.

IT 222978-91-8P

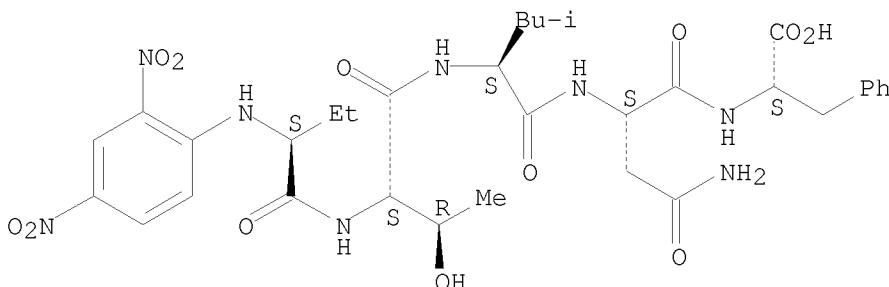
RL: BYP (Byproduct); PREP (Preparation)

(solid-phase peptide synthesis by fragment condensation coupling in swelling volume)

RN 222978-91-8 HCPLUS

CN L-Phenylalanine, (2S)-2-[(2,4-dinitrophenyl)amino]butanoyl-L-threonyl-L-leucyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 28 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1999:77546 HCPLUS

DOCUMENT NUMBER: 130:158261

TITLE: Novel oxidative hair dye compositions containing cationic oxidation bases

INVENTOR(S): Genet, Alain; Lagrange, Alain

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: PCT Int. Appl., 72 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9903836	A1	19990128	WO 1998-FR1535	19980713
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2766178	A1	19990122	FR 1997-9028	19970716
FR 2766178	B1	20000317		
CA 2265539	A1	19990128	CA 1998-2265539	19980713
CA 2265539	C	20050215		
AU 9887355	A	19990210	AU 1998-87355	19980713
EP 928289	A1	19990714	EP 1998-938745	19980713
EP 928289	B1	20040929		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000503037	T	20000314	JP 1999-506576	19980713
JP 3825056	B2	20060920		
AT 277908	T	20041015	AT 1998-938745	19980713
ES 2230708	T3	20050501	ES 1998-938745	19980713
US 6638321	B1	20031028	US 1999-254663	19990607
PRIORITY APPLN. INFO.:				
			FR 1997-9028	A 19970716
			WO 1998-FR1535	W 19980713

## ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 130:158261

AB Novel monobenzene oxidation bases comprise at least a cationic group being selected among the aliphatic chains containing at least a quaternized unsatd. cycle. Their use for oxidation dyeing of keratin fibers, dyeing compns. containing them and oxidation dyeing methods using them is disclosed. Thus, 1-[2-(4-aminophenylamino)-ethyl]-3-methyl-3H-imidazol-1-ium (I) was prepared by reduction of 3-methyl-1-[2-(4-nitrophenylamino)-ethyl]-3H-imidazol-1-ium and reaction with HCl. A hair dye preparation contained I 1.036, 2-methyl-5-N-( $\beta$ -hydroxyethyl)aminophenol 0.543 and excipient q.s. 100 g.

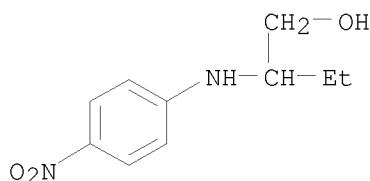
IT 220159-25-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel oxidative hair dye compns. containing cationic oxidation bases)

RN 220159-25-1 HCAPLUS

CN 1-Butanol, 2-[(4-nitrophenyl)amino]- (CA INDEX NAME)

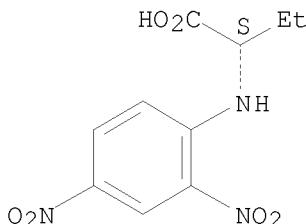


OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS RECORD (25 CITINGS)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1998:491329 HCAPLUS  
 DOCUMENT NUMBER: 129:197343  
 ORIGINAL REFERENCE NO.: 129:39901a,39904a  
 TITLE: Highly enantioselective HPLC separations using the covalently bonded macrocyclic antibiotic, ristocetin A, chiral stationary phase  
 AUTHOR(S): Ekborg-Ott, K.; Liu, Youbang; Armstrong, Daniel W.  
 CORPORATE SOURCE: Department Chemistry, University Missouri-Rolla, Rolla, MO, USA  
 SOURCE: Chirality (1998), 10(5), 434-483  
 CODEN: CHRLEP; ISSN: 0899-0042  
 PUBLISHER: Wiley-Liss, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The macrocyclic glycopeptide, ristocetin A, was covalently bonded to a silica gel support and evaluated as a liquid chromatog. (LC) chiral stationary phase (CSP). Over 230 racemates were resolved in either the reversed-phase mode, the normal-phase mode, or the polar-organic mode. The retention behavior and selectivity of this CSP were examined in each mode. Optimization of sepn. on this column is discussed. The ristocetin A CSP appeared to be complimentary to other glycopeptide CSPs (i.e., vancomycin and teicoplanin). Column stability was excellent. The CSP was not irreversibly altered when going from one mobile phase mode to another.  
 IT 4470-69-3  
 RL: ANT (Analyte); PEP (Physical, engineering or chemical process); PRP (Properties); ANST (Analytical study); PROC (Process)  
 (enantiomeric separation by HPLC using covalently bonded macrocyclic antibiotic ristocetin A as chiral stationary phase)  
 RN 4470-69-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 109 THERE ARE 109 CAPLUS RECORDS THAT CITE THIS RECORD (110 CITINGS)  
 REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 30 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1998:208450 HCAPLUS  
 DOCUMENT NUMBER: 128:267960  
 ORIGINAL REFERENCE NO.: 128:52979a,52982a  
 TITLE: Crosslinked protein crystals as universal separation media

INVENTOR(S): Margolin, Alexey L.; Vilenchik, Lev Z.  
 PATENT ASSIGNEE(S): Altus Biologics Inc., USA; Margolin, Alexey L.;  
 Vilenchik, Lev Z.  
 SOURCE: PCT Int. Appl., 115 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9813119	A1	19980402	WO 1997-US17167	19970924
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9747381	A	19980417	AU 1997-47381	19970924
PRIORITY APPLN. INFO.:			US 1996-719114	A2 19960924
			WO 1997-US17167	W 19970924

AB The present invention relates to the use of crosslinked protein crystals in methods, apparatus and systems for separating a substance or mol. of interest

from a sample. According to a preferred embodiment of this invention, crosslinked protein crystals are used in chromatog. methods, apparatus and systems in which separation is based on a phys. or chemical property of that substance or mol. of interest. Advantageously, the crosslinked protein crystals which characterize the methods, apparatus and systems of this invention possess excellent mech. strength and well developed porous structure, demonstrate significant affinity and chiral selectivity and are extremely stable in aqueous and organic solvents. These properties render the crystals particularly useful as sorbents for sepn., including size exclusion, affinity and chiral chromatog. Crosslinked bovine serum albumin crystals were prepared and packed in a chromatog. column.

Ketoprofen, suprofen, and naproxen were separated by affinity chromatog.

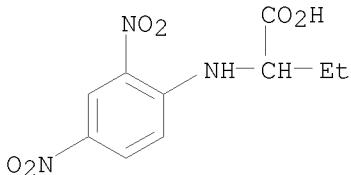
IT 31356-29-3P

RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical study); PREP (Preparation)

(crosslinked protein crystals as universal separation media)

RN 31356-29-3 HCPLUS

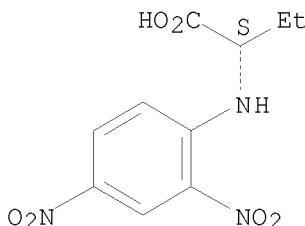
CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



REFERENCE COUNT: 6 RECORD (10 CITINGS)  
 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 31 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1998:106701 HCPLUS  
 DOCUMENT NUMBER: 128:135908  
 ORIGINAL REFERENCE NO.: 128:26545a, 26548a  
 TITLE: Characterization and Evaluation of d-(+)-Tubocurarine Chloride as a Chiral Selector for Capillary Electrophoretic Enantioseparations  
 AUTHOR(S): Nair, Usha B.; Armstrong, Daniel W.; Hinze, Willie L.  
 CORPORATE SOURCE: Departments of Chemistry, University of Missouri-Rolla, Rolla, MO, 65401, USA  
 SOURCE: Analytical Chemistry (1998), 70(6), 1059-1065  
 CODEN: ANCHAM; ISSN: 0003-2700  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A new macrocyclic of the bis(benzylisoquinoline) alkaloid family, d-(+)-tubocurarine chloride (DTC), was evaluated as a chiral selector for the separation of optical isomers of organic carboxylates using capillary electrophoresis (CE). The pertinent physicochem. properties, such as absorption spectrum, isoionic point, and solution conformation, of DTC were determined. The effects varying such exptl. parameters as DTC concentration, pH, and methanol content in the running buffer were assessed. CE separation of the enantiomers of 18 different compds. was achieved using DTC as the chiral selector under optimized background electrolytic conditions.  
 IT 4470-69-3, L-(2,4-Dinitrophenyl)- $\alpha$ -amino-n-butyric acid  
 RL: ANT (Analyte); ANST (Analytical study)  
 (organic carboxylate enantiomers resolution by capillary electrophoresis using tubocurarine chloride as chiral selector)  
 RN 4470-69-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

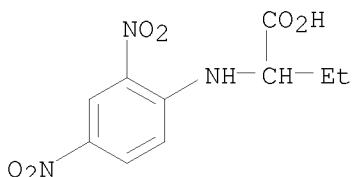
Absolute stereochemistry.



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)  
 REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 32 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1997:748872 HCPLUS  
 DOCUMENT NUMBER: 128:97110

ORIGINAL REFERENCE NO.: 128:18833a,18836a  
TITLE: Evaluation of two amine-functionalized cyclodextrins as chiral selectors in capillary electrophoresis: comparisons to vancomycin  
AUTHOR(S): Nair, Usha B.; Armstrong, Daniel W.  
CORPORATE SOURCE: Department of Chemistry, University of Missouri, Rolla, MO, 65401, USA  
SOURCE: Microchemical Journal (1997), 57(2), 199-217  
CODEN: MICJAN; ISSN: 0026-265X  
PUBLISHER: Academic Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Two different amine-functionalized  $\beta$ -cyclodextrins were evaluated as chiral selectors in capillary electrophoresis. The first was a monosubstituted 6-ethylenediamine-derivatized  $\beta$ -cyclodextrin, and the other was quaternary ammonium hydroxypropyl- $\beta$ -cyclodextrin. The former compound was more widely useful as a chiral selector and had less effect on the electroosmotic flow than the latter compound. Both tended to resolve anionic compds. The primary attractive interaction between these host chiral selectors and their enantiomeric guests were charge-charge (ionic) and hydrophobic inclusion. Addnl. interactions involved hydrogen bonding and/or steric repulsions. The cationic cyclodextrins were not as widely useful in resolving anionic compds. as was vancomycin. However, they tended to be more stable and were comparatively transparent to near-UV light.  
IT 31356-29-3, 2,4-Dinitrophenyl-DL- $\alpha$ -amino-n-butyric acid  
RL: ANT (Analyte); ANST (Analytical study)  
(chiral resolution of; chiral selection mechanisms and ability of amine-functionalized cyclodextrins in capillary electrophoresis)  
RN 31356-29-3 HCPLUS  
CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)  
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 33 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1997:476570 HCAPLUS  
DOCUMENT NUMBER: 127:220944  
ORIGINAL REFERENCE NO.: 127:43069a  
TITLE: A nonempirical method using LC/MS for determination of the absolute configuration of constituent amino acids in a peptide: elucidation of limitations of Marfey's method and of its separation mechanism  
AUTHOR(S): Fujii, Kiyonaga; Ikai, Yoshitomo; Mayumi, Tsuyoshi; Oka, Hisao; Suzuki, Makoto; Harada, Ken-ichi

CORPORATE SOURCE: Faculty of Pharmacy, Meijo University, Tempaku, 468, Japan

SOURCE: Analytical Chemistry (1997), 69(16), 3346-3352  
CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB As the first step in establishing the author's proposed method, the advanced Marfey's method, which is planned for the simultaneous determination of

the absolute configuration of amino acids in a peptide, Marfey's method was applied to com. available amino acids, and the separation behavior was examined in detail. Although good resolution of the diastereomeric pair of an individual amino acid was obtained for all amino acids tested and the applicability of the method was confirmed, the (1-fluoro-2,4-dinitrophenyl)-5-L-alaninamide (FDAA) derivative of the L-amino acid was not always eluted prior to its corresponding D-amino acid derivative. Because this proposed method relies on the elution order of a derivatized amino acid with FDAA to determine its absolute configuration, its separation mechanism

was carefully investigated using UV and NMR spectral techniques. The results suggested that the resulting conformations of the L- and D-amino acid derivs. are stable and that the resolution between the L- and D-amino acid derivs. is due to the difference in their hydrophobicity, which is derived from the cis- or trans-type arrangement of two more hydrophobic substituents at both  $\alpha$ -carbons of an amino acid and L-alanine amide, so that the FDAA derivative of the cis (Z)-type arrangement interacts more strongly with ODS silica gel and has a longer retention time than that of the trans (E)-type arrangement. Therefore, the L-amino acid derivative is usually eluted from the column before its corresponding D-amino acid derivative in Marfey's method. According to this separation mechanism, the elution

order of a desired amino acid can be elucidated from the average retention time of the L- and D-amino acid derivs., and the DL-serine and DL-asparagine derivs. are critical for Marfey's method.

IT 194736-16-8P

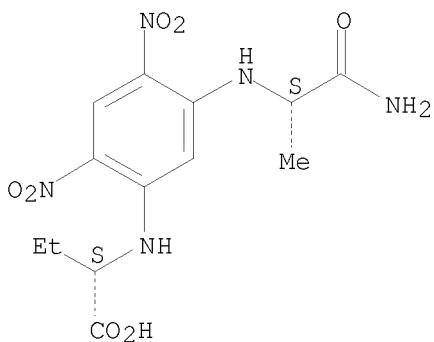
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(nonempirical method using LC/MS for determination of the absolute configuration of

constituent amino acids in peptides)

RN 194736-16-8 HCPLUS

CN Butanoic acid, 2-[(5-[(1S)-2-amino-1-methyl-2-oxoethyl]amino]-2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

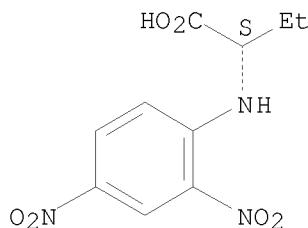


OS.CITING REF COUNT: 92 THERE ARE 92 CAPLUS RECORDS THAT CITE THIS RECORD (92 CITINGS)  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

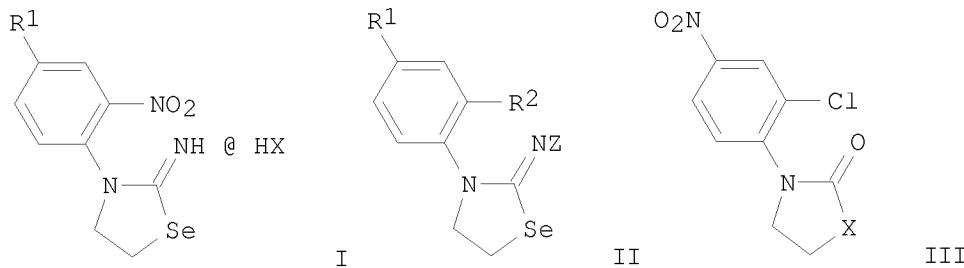
L11 ANSWER 34 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1997:126060 HCAPLUS  
 DOCUMENT NUMBER: 126:238564  
 ORIGINAL REFERENCE NO.: 126:46169a, 46172a  
 TITLE: Preparation of a  $\beta$ -cyclodextrin-modified N-carboxymethylchitosan and its chromatographic behavior as a chiral HPLC stationary phase  
 AUTHOR(S): Kurauchi, Yoshiaki; Ono, Hiroyoshi; Wang, Bo; Egashira, Naoyoshi; Ohga, Kazuya  
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Oita University, Oita, 870-11, Japan  
 SOURCE: Analytical Sciences (1997), 13(1), 47-52  
 CODEN: ANSCEN; ISSN: 0910-6340  
 PUBLISHER: Japan Society for Analytical Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Chitosan, whose deacetylation degree was 0.95, was N-carboxymethylated and subsequently modified with 6-amino-6-deoxy- $\beta$ -cyclodextrin. The  $^1\text{H}$  NMR spectra of the carboxymethylated chitosan (NCMC) and the  $\beta$ -cyclodextrin-modified NCMC ( $\beta$ -CD-NCMC) showed introductions of ca. 8.4 of the carboxymethyl groups and 8.2 of  $\beta$ -CD moieties per 10 units, resp.  $\beta$ -CD-NCMC was covalently attached to a macroporous silica gel and used as a stationary phase for chiral HPLC sepns. of 2,4-dinitrophenyl- $\alpha$ -amino acids and related racemates. The chiral discrimination was influenced more strongly by the size of an alkyl group on the chiral center of the aliphatic amino acids, compared to a Cyclobond I bearing monomeric  $\beta$ -CD mols. The distance between two aromatic moieties on the aromatic amino acids and related racemates was also discriminated. The strict recognition required the high substitution degree of the  $\beta$ -CD moiety, permitting us to propose a simultaneous inclusion of the 2,4-dinitrophenyl group and another aromatic substituent or an alkyl group with a proper size into the two adjacent CD cavities on the polymer chain.  
 IT 4470-69-3P  
 RL: PUR (Purification or recovery); PREP (Preparation)  
 (preparation of a  $\beta$ -cyclodextrin-modified N-carboxymethylchitosan and its chromatog. behavior as a chiral HPLC stationary phase)  
 RN 4470-69-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)

L11 ANSWER 35 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1996:426976 HCAPLUS  
 DOCUMENT NUMBER: 125:195846  
 ORIGINAL REFERENCE NO.: 125:36687a, 36690a  
 TITLE: Synthesis, some reactions and anti-ulcer activity of some 2-amino-3-(substituted phenyl)selenazolidines  
 AUTHOR(S): Hornyak, Gyula; Feller, Antal; Lempert, Karoly  
 CORPORATE SOURCE: Res. Group Alkaloid Chem., Hungarian Academy Sci., Budapest, H-1521, Hung.  
 SOURCE: ACH - Models in Chemistry (1995), 132(6), 871-885  
 CODEN: ACMCEI; ISSN: 1217-8969  
 PUBLISHER: Akademiai Kiado  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 125:195846  
 GI



AB 2-Imino-3-(substituted phenyl)selenazolidine salts, e.g., I (R1 = H, NO2, CF3, X = Cl, Br), were prepared (1) by acid induced ring closure of N-(2-selenocyanatoethyl)anilines, or (2) by fusion of anilines with 2-bromoethylselenocyanate. E.g., 2-NO2C6H4NHCH2CH2SeCN is refluxed in dioxane the presence of ethanesulfonic acid to give I (R1 = H, HX = HO3SET) in 93% yield. Diselenide, e.g., (ArNHCH2CH2Se)2, formation accompanying the syntheses according to Method 1 above was successfully suppressed. Some N-substituted derivs. (e.g., II, R1 ≠ R2 = Cl,

NO<sub>2</sub>, Z = CHO, Ac, CONHPr, SO<sub>2</sub>Et) of selenazolidines I, as well as 3-aryl-selenazolidin-2-one III (X = Se), and its thiazolidinone analog III (X = S), were also prepared. The gastroprotective (antiulcer) activity of some of I, II and III is reported.

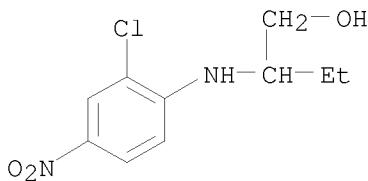
IT 180691-77-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methylsulfonylation in the synthesis of amino(substituted phenyl)selenazolidines as antiulcer agents)

RN 180691-77-4 HCPLUS

CN 1-Butanol, 2-[(2-chloro-4-nitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 36 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1996:357976 HCPLUS

DOCUMENT NUMBER: 125:131259

ORIGINAL REFERENCE NO.: 125:24261a

TITLE: Chiral separation of  $\alpha$ -amino acid derivatives by capillary electrophoresis using 6-amino-6-deoxy- $\beta$ -cyclodextrin and its N-hexyl derivative as chiral selectors

AUTHOR(S): Egashira, Naoyoshi; Mutoh, Osamu; Kurauchi, Yoshiaki; Ohga, Kazuya

CORPORATE SOURCE: Department Applied Chemistry, Oita University, Oita, 870-11, Japan

SOURCE: Analytical Sciences (1996), 12(3), 503-505  
CODEN: ANSCEN; ISSN: 0910-6340

PUBLISHER: Japan Society for Analytical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The chiral seprns. of N-(2,4-dinitrophenyl)- and N-dansyl- $\alpha$ -amino acids by capillary zone electrophoresis (CZE) using 6-amino-6-deoxy- $\beta$ -cyclodextrin (ACD) and 6-deoxy-6-hexylamino- $\beta$ -cyclodextrin (HACD) as chiral selectors. Tetraalkylammonium additives with short alkyl chains adsorbed on a capillary silica wall have improved in CZE through controlling an electroosmotic flow. ACD having an amino group is also expected to adsorb on the capillary silica wall, and, thus, to produce more effective chiral separation. Further, chiral seprns. with HACD have been compared to those with ACD on the basis of the hydrophobicity of the hexyl group on HACD.

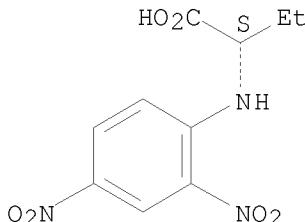
IT 4470-69-3

RL: ANT (Analyte); ANST (Analytical study)  
(chiral separation of  $\alpha$ -amino acid derivs. by capillary electrophoresis using 6-amino-6-deoxy- $\beta$ -cyclodextrin and its N-hexyl derivative as chiral selectors)

RN 4470-69-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

L11 ANSWER 37 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1996:356933 HCAPLUS

DOCUMENT NUMBER: 125:167832

ORIGINAL REFERENCE NO.: 125:31449a,31452a

TITLE: Synthesis of new pyrrolo- and thieno[2,3-b]pyridine derivatives by the Thorpe-Ziegler reaction

AUTHOR(S): Yakovlev, M. Yu.; Kadushkin, A. V.; Granik, V. G.

CORPORATE SOURCE: TsKhLS-VNIKhFI, Moscow, Russia

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1996), 30(2), 36-38

CODEN: KHFZAN; ISSN: 0023-1134

PUBLISHER: Izdatel'stvo Foliom

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 125:167832

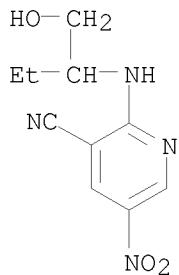
AB Various 2-aminopyridines were prepared in good yields by reacting 2-chloro-3-cyano-5-nitropyridine with amines and amino alcs. The product of the reaction with glycine Me ester, 2-[(methoxycarbonyl)methyl]amino]-3-cyano-5-nitropyridine, failed to enter the Thorpe-Ziegler cyclization, presumably due to the presence of the secondary amino group. The reaction with N-methylaminoacetate and thioglycolate gave suitable intermediates, which in the presence of Na ethoxide underwent intermol. Thorpe-Ziegler cyclization to afford pyrrolo- and thieno[2,3-b]pyridines.

IT 180424-16-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of pyrrolo- and thieno[2,3-b]pyridines by Thorpe-Ziegler cyclization)

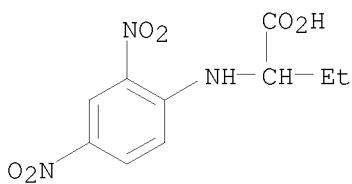
RN 180424-16-2 HCAPLUS

CN 3-Pyridinecarbonitrile, 2-[(1-hydroxymethyl)propyl]amino]-5-nitro- (CA INDEX NAME)



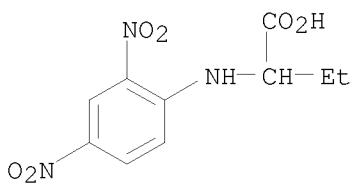
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(4 CITINGS)

L11 ANSWER 38 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1996:148859 HCAPLUS  
 DOCUMENT NUMBER: 124:242482  
 ORIGINAL REFERENCE NO.: 124:44713a, 44716a  
 TITLE: Capillary electrophoretic enantiomeric separations using the glycopeptide antibiotic, teicoplanin  
 AUTHOR(S): Rundlett, Kimber L.; Gasper, Mary P.; Zhou, Eve Y.; Armstrong, Daniel W.  
 CORPORATE SOURCE: University Missouri, Rolla, MO, USA  
 SOURCE: Chirality (1996), 8(1), 88-107  
 CODEN: CHRLEP; ISSN: 0899-0042  
 PUBLISHER: Wiley-Liss  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Teicoplanin is the third in a series of macrocyclic glycopeptide antibiotics that has been evaluated as a chiral selector in capillary electrophoresis (CE). It was used to resolve over 100 anionic racemates at low selector concns. Like the other related glycopeptide antibiotics, its enantioselectivity tends to be opposite to that of the ansa-type antibiotics which prefers cationic compds., particularly amines. Factors that affect teicoplanin-based enantiosepsns. include the selector as well as the enantiosepn. Teicoplanin exhibited some features that were not noted with the other glycopeptide antibiotics. it forms micelles in aqueous solns. and this influence its enantioselectivity. Unlike the other studied glycopeptides, teicoplanin ppts. in alc.-water mixts. It also binds less to the capillary wall than vancomycin as evidenced by the faster electroosmotic flow velocity. The micellization of teicoplanin is pH dependent so that the effect of pH on enantiorecognition is more complex for teicoplanin than for other chiral selectors. Also it is shown that the simple model proposed to explain the role of organic modifiers in cyclodextrin-based CE enantiosepsns. may not apply to these and other systems.  
 IT 31356-29-3  
 RL: ANT (Analyte); ANST (Analytical study)  
 (enantiomeric separation of drugs by capillary electrophoresis using teicoplanin as a chiral selector)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 77 THERE ARE 77 CAPLUS RECORDS THAT CITE THIS RECORD (77 CITINGS)

L11 ANSWER 39 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1995:320833 HCAPLUS  
 DOCUMENT NUMBER: 122:142711  
 ORIGINAL REFERENCE NO.: 122:26343a, 26346a  
 TITLE: Highly enantioselective capillary electrophoretic separations with dilute solutions of the macrocyclic antibiotic ristocetin A  
 AUTHOR(S): Armstrong, Daniel W.; Gasper, Mary P.; Rundlett, Kimber L.  
 CORPORATE SOURCE: Department of Chemistry, University of Missouri-Rolla, Rolla, MO, 65401, USA  
 SOURCE: Journal of Chromatography, A (1995), 689(2), 285-304  
 CODEN: JCRAEY; ISSN: 0021-9673  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Ristocetin A is one of a series of structurally related amphoteric, glycopeptide, macrocyclic antibiotics. These compds. have several features that make them attractive as chiral selectors. These include spatially oriented functional groups that are known to provide the types of interactions that are conducive to enantio-recognition, a somewhat rigid "pocket" that can provide a site for hydrophobic interactions and polar, flexible arms (i.e., pendent sugar moieties) that can rotate to hydrogen bond and otherwise interact with a variety of chiral analytes. In addition, these compds. are sufficiently soluble in water, aqueous buffers and aqueous-organic solvents that are commonly used in capillary electrophoresis (CE). The use and optimization of ristocetin A as a chiral selector in CE is discussed. Over 120 racemates are resolved including a variety of N-blocked amino acids, non-steroidal anti-inflammatory compds. and a large number of biol. important compds. containing carboxylic acid groups (e.g., mandelic acid derivs., lactic acid derivs., folic acid, tropic acid).  
 IT 31356-29-3P  
 RL: PUR (Purification or recovery); PREP (Preparation)  
 (highly enantioselective capillary electrophoretic sepns. with dilute solns. of the macrocyclic antibiotic ristocetin A)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)

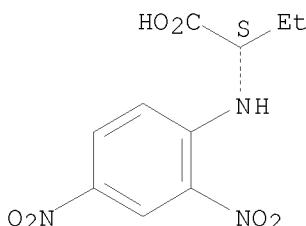


OS.CITING REF COUNT: 106 THERE ARE 106 CAPLUS RECORDS THAT CITE THIS RECORD (107 CITINGS)

L11 ANSWER 40 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1995:111539 HCAPLUS  
 DOCUMENT NUMBER: 123:24944  
 ORIGINAL REFERENCE NO.: 123:4403a, 4406a  
 TITLE: Evaluation of the macrocyclic antibiotic vancomycin as a chiral selector for capillary electrophoresis  
 AUTHOR(S): Armstrong, Daniel W.; Rundlett, Kimber L.; Chen, Jing-Ran  
 CORPORATE SOURCE: Dep. Chem., Univ. Missouri-Rolla, Rolla, MO, USA  
 SOURCE: Chirality (1994), 6(6), 496-509  
 CODEN: CHRLEP; ISSN: 0899-0042  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Vancomycin is one of a family of related macrocyclic glycopeptide antibiotics that were discovered by the scientists at the Eli Lilly Company in the 1950s. It has been used to treat severe staphylococcal infections, particularly when bacterial resistance to other antibiotics has developed. Vancomycin is a naturally occurring chiral compound and has a number of stereogenic centers. Furthermore, it contains a variety of functionalities that are known to be useful for enantioselective interactions (e.g., hydrogen bonding groups, hydrophobic pockets, aromatic groups, amide linkages, etc.). The physicochem. properties of vancomycin, including its stability in solution, are discussed as they pertain to capillary electrophoresis. Over 100 racemates were resolved including many nonsteroidal antiinflammatory drugs, antineoplastic compds. and N-derivatized amino acids. Many of these compds. had very high resolution factors. Optimization and the effect of different exptl. parameters on the enantioselective sepns. are discussed.

IT 4470-69-3  
 RL: ANT (Analyte); ANST (Analytical study)  
 (evaluation of macrocyclic antibiotic vancomycin as chiral selector for capillary electrophoresis)  
 RN 4470-69-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

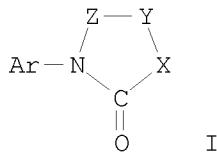
Absolute stereochemistry.



OS.CITING REF COUNT: 193 THERE ARE 193 CAPLUS RECORDS THAT CITE THIS RECORD (195 CITINGS)

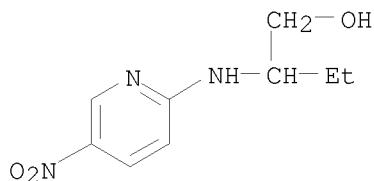
L11 ANSWER 41 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1994:545848 HCAPLUS  
 DOCUMENT NUMBER: 121:145848  
 ORIGINAL REFERENCE NO.: 121:26141a, 26144a  
 TITLE: heterocyclic compound crystals and manufacture thereof  
 INVENTOR(S): Komatsu, Hiromi; Shigemoto, Takeo; Sugiyama, Tsunetoshi  
 PATENT ASSIGNEE(S): Japan Synthetic Rubber Co Ltd, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06056771	A	19940301	JP 1992-233134	19920807
PRIORITY APPLN. INFO.:			JP 1992-233134	19920807
OTHER SOURCE(S):	MARPAT	121:145848		
GI				

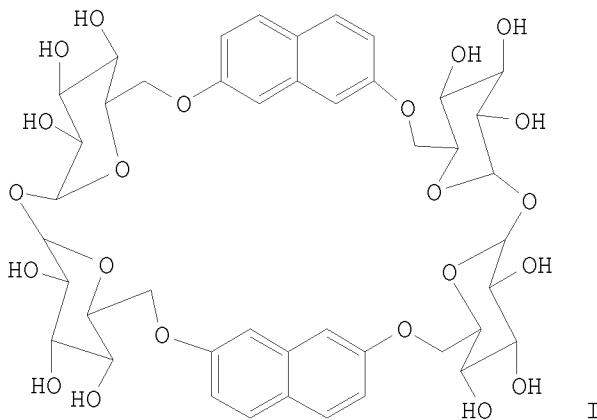


AB The crystal is represented by I (X, Y, Z=C, O, S, or N with optional substituting H, or monovalent or divalent radical except for O atom(s); Ar=aromatic radical with optional substituting radical(s)) and has  $\geq 1$  pairs of optically even faces parallel to each other. A solvent(s) which have solubility of 1-50 g at 25° may be used for growth, and may be a mixture of  $\geq 2$  solvents such that crystal habit of the crystal grown from a single solvent differs from that from the other solvent.

IT 149873-63-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, oxazolidinone derivative compds. from)  
 RN 149873-63-2 HCAPLUS  
 CN 1-Butanol, 2-[(5-nitro-2-pyridinyl)amino]- (CA INDEX NAME)



L11 ANSWER 42 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1994:134962 HCAPLUS  
 DOCUMENT NUMBER: 120:134962  
 ORIGINAL REFERENCE NO.: 120:23799a,23802a  
 TITLE: Glycophanes, cyclodextrin-cyclophane hybrid receptors for apolar binding in aqueous solutions. A stereoselective carbohydrate-carbohydrate interaction in water  
 AUTHOR(S): Coteron, Jose M.; Vicent, Cristina; Bosso, Claude; Penades, Soledad  
 CORPORATE SOURCE: Inst. Quim. Org., CSIC, Madrid, 28006, Spain  
 SOURCE: Journal of the American Chemical Society (1993), 115(22), 10066-76  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The synthesis and complexing properties of a new type of neutral chiral receptors, cyclodextrin-cyclophanes, e.g. I, are reported. They are built from  $\alpha,\alpha'$ -trehalose and 2,7-dihydroxynaphthalene or 4,4'-isopropylidenediphenol. The water soluble glycophane I displays a general affinity for electron-deficient aromatic guests (nitro derivs. of phenol and benzenesulfonic and benzenecarboxylic acids), the association consts. increasing with the increased number of electron-withdrawing groups (NO<sub>2</sub>). Depending on the solvent, different factors seem to contribute to the stability of the complexes. In CD<sub>3</sub>OD:D<sub>2</sub>O (1:1), electron donor-acceptor interactions are the main driving forces, whereas in water, addnl. hydrophobic effects increase the stability of the complexes. Glycophane I shows chiral discrimination toward racemic mixts. of 2,4-dinitrophenyl amino acid derivs. in solid-liquid extraction expts., with enantioselectivities ranging from 2,4-dinitrophenyl amino acid derivs. in solid-liquid extraction expts., with enantioselectivities ranging from 5 to 40% as deduced by integration of the aromatic proton NMR signals of both enantiomers. Cyclodextrins (CDs) under the same conditions did not show any discrimination toward these derivs. A stereospecific

carbohydrate-carbohydrate interaction in water has been shown between glycophane I and the 4-nitrophenyl  $\alpha$ - and  $\beta$ -D-glucosyl,  $\alpha$ - and  $\beta$ -D-galactosyl, and  $\alpha$ - and  $\beta$ -D-mannopyranosyl derivs., and the contribution of this interaction to complex stability has been evaluated. The complexes of CDs and 4-nitrophenyl glycosides did not show any addnl. stabilization due to carbohydrate moieties.

IT 152866-65-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 152866-65-4 HCPLUS

CN  $\alpha$ -D-Glucopyranoside, 6,6':6',6'''-bis-0-2,7-naphthalenediylbis[ $\alpha$ -D-glucopyranosyl, compd. with (R)-2-[(2,4-dinitrophenyl)amino]butanoic acid (1:1) (9CI) (CA INDEX NAME)

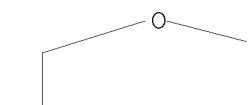
CM 1

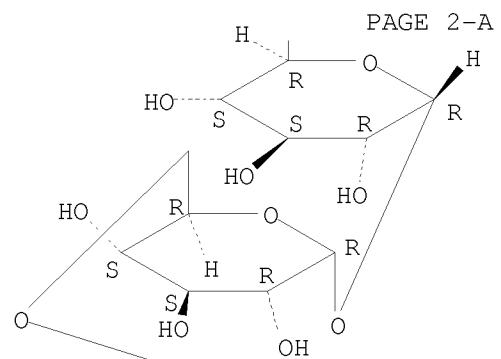
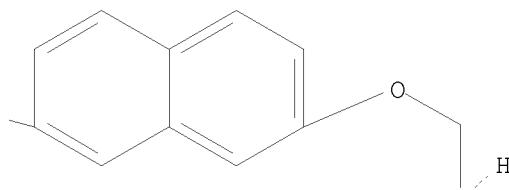
CRN 142409-32-3

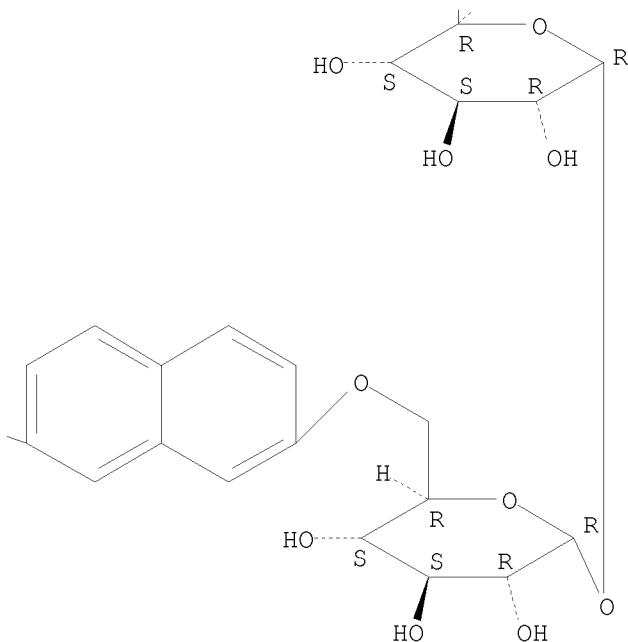
CMF C44 H52 O22

Absolute stereochemistry.

PAGE 1-A



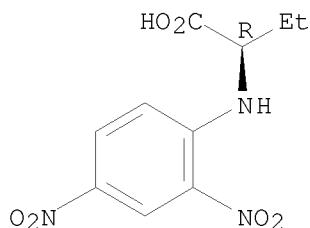




CM 2

CRN 6367-34-6  
CMF C10 H11 N3 O6

Absolute stereochemistry.



OS.CITING REF COUNT: 59 THERE ARE 59 CAPLUS RECORDS THAT CITE THIS RECORD (59 CITINGS)

L11 ANSWER 43 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1993:594750 HCAPLUS  
 DOCUMENT NUMBER: 119:194750  
 ORIGINAL REFERENCE NO.: 119:34473a, 34476a  
 TITLE: Thin-layer chromatographic enantioseparation of  
 miscellaneous compounds with bovine serum albumin in  
 the eluent  
 AUTHOR(S): Lepri, Luciano; Coas, Vanda; Desideri, Pier Giorgio;  
 Pettini, Lilia  
 CORPORATE SOURCE: Dep. Public Health, Epidemiol., Univ. Florence,

SOURCE: Florence, 50121, Italy  
 Journal of Planar Chromatography--Modern TLC (1993),  
 6(2), 100-4  
 CODEN: JPCTE5; ISSN: 0933-4173

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The enantiomers of several optically active organic compds. have been separated using optimized chromatog. systems comprising RP-18W/UV254 or Sil C18-50 UV254 layers and eluents of different pH and ionic strength containing different amts. of bovine serum albumin (BSA) and organic modifier. BSA shows high enantioselectivity towards different N derivs. of DL amino acids, fluoro substituted tryptophans, and finally, unusual enantiomers such as 1,1'-bi-2-naphthol, binaphthyl-2,2'-diyl hydrogen phosphate,  $\beta$ -hydrastine, p-nitrophenyl- $\beta$ -thiopyranoside, and 3,5-dinitro-N-(1-phenylethyl)benzamide, never before separated with this chiral agent. A total of more than 75 racemates has been separated in the authors' expts. with planar chromatog. using BSA in the mobile phase [reported in this and previous work] and the data obtained furnish some interesting suggestions which might serve as a guideline for chiral sepn.

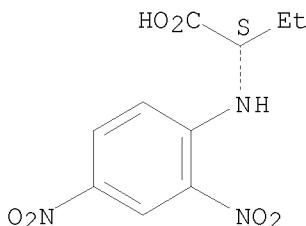
IT 4470-69-3

RL: ANT (Analyte); ANST (Analytical study)  
 (thin-layer chromatog. of, with bovine serum albumin-containing eluent)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



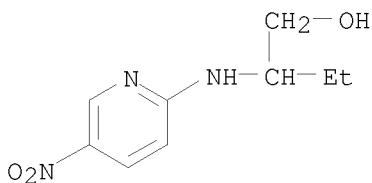
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

L11 ANSWER 44 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1993:570229 HCPLUS  
 DOCUMENT NUMBER: 119:170229  
 ORIGINAL REFERENCE NO.: 119:30265a,30268a  
 TITLE: Nonlinear optical device  
 INVENTOR(S): Shigemoto, Takeo; Sugiyama, Tsunetoshi; Ukaji, Takashi  
 PATENT ASSIGNEE(S): Japan Synthetic Rubber Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 32 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

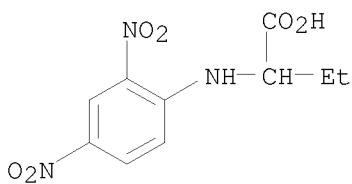
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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## STN Search

JP 05045688 A 19930226 JP 1991-289294 19911008  
 PRIORITY APPLN. INFO.: MARPAT 119:170229 JP 1990-295110 A1 19901031  
 OTHER SOURCE(S):  
 AB The title device consists of a compound XCH<sub>2</sub>C(R)HNHA [R (un)substituted alkyl, alkenyl, alkynyl, aryl, aralkyl, acyl, CO<sub>2</sub>H, carbamoyl, YS<sub>1</sub>CH<sub>2</sub>; Y = benzyl, C<sub>14</sub> alkyl; X = OH, alkoxy, aralkyloxy; A = (un)substituted (hetero)aromatic] or a polymer containing the compound chemical bonded to the polymer.  
 IT 149873-63-2P  
 RL: PREP (Preparation)  
 (preparation of, as nonlinear optical material)  
 RN 149873-63-2 HCPLUS  
 CN 1-Butanol, 2-[(5-nitro-2-pyridinyl)amino]- (CA INDEX NAME)



L11 ANSWER 45 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1993:246573 HCPLUS  
 DOCUMENT NUMBER: 118:246573  
 ORIGINAL REFERENCE NO.: 118:42521a, 42524a  
 TITLE: Direct separation of enantiomers using multiple-interaction chiral stationary phases based on the modified  $\beta$ -cyclodextrin-bonded stationary phase  
 AUTHOR(S): Li, Song; Purdy, William C.  
 CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3A 2K6, Can.  
 SOURCE: Journal of Chromatography (1992), 625(2), 109-20  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Several multiple-interaction chiral stationary phases have been developed. These stationary phases contain a hydrophobic cavity capable of inclusion complexation, aromatic groups capable of  $\pi$ - $\pi$  interaction, polar hydroxyl groups capable of hydrogen-bonding with the polar functional groups of the solute, and bulky non-polar groups providing steric repulsion. The characteristics and properties of these stationary phases are described. The direct separation of enantiomers of a wide variety of chiral compds. are reported. The effect of mobile phase composition on the retention and resolution is discussed.  
 IT 31356-29-3  
 RL: ANST (Analytical study); PROC (Process)  
 (resolution of, by HPLC on modified  $\beta$ -cyclodextrin-bonded stationary phase)  
 RN 31356-29-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)

L11 ANSWER 46 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1988:187273 HCAPLUS  
 DOCUMENT NUMBER: 108:187273  
 ORIGINAL REFERENCE NO.: 108:30791a, 30794a  
 TITLE: Optical resolution of amino acids  
 INVENTOR(S): Yuasa, Seiji  
 PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62070348	A	19870331	JP 1985-210313	19850925
JP 06013463	B	19940223		

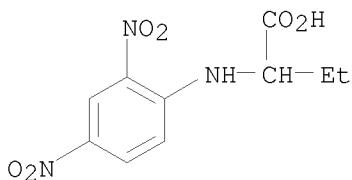
PRIORITY APPLN. INFO.: JP 1985-210313 19850925

AB Mixts. of D- and L-amino acids are resolved by transforming to N-(substituted aryl) derivs. and separating by liquid chromatograph. Thus, an aqueous solution of racemic isoleucine and NaHCO3 was treated with 2,4-(O2N)2C6H3F in EtOH at 80° to give the N-aryl derivs., which were separated on a cellulose column using BuOH/EtOH/H2O (4/1/0.1 vol) as eluent. The separation factor was 2.23.

IT 31356-29-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and optical resolution of, by liquid chromatog.)

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L11 ANSWER 47 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1985:407732 HCAPLUS

## STN Search

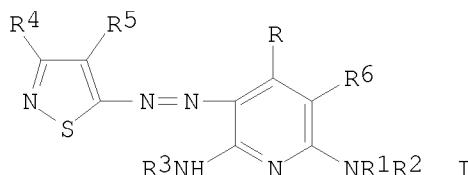
DOCUMENT NUMBER: 103:7732  
 ORIGINAL REFERENCE NO.: 103:1373a, 1376a  
 TITLE: Isothiazole azo dyes  
 INVENTOR(S): Loeffler, Hermann; Schefczik, Ernst  
 PATENT ASSIGNEE(S): BASF A.-G. , Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 25 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3330155	A1	19850307	DE 1983-3330155	19830820
EP 135131	A1	19850327	EP 1984-109602	19840813
EP 135131	B1	19861105		
R: CH, DE, FR, GB, IT, LI				
JP 60065066	A	19850413	JP 1984-171675	19840820
US 4774324	A	19880927	US 1986-838195	19860307
PRIORITY APPLN. INFO.:			DE 1983-3330155	A 19830820
			US 1984-641580	A2 19840817

## ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 103:7732

GI



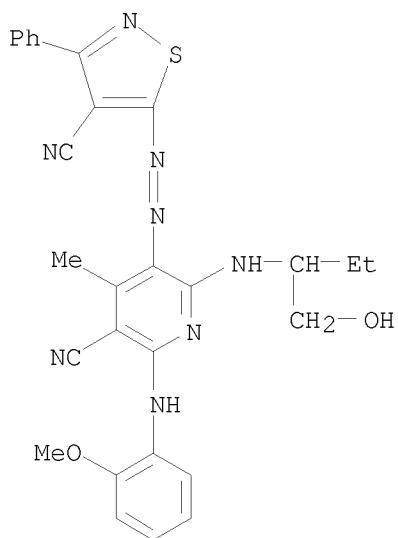
AB Title dyes of general structure I are prepared, where R = H, C1-3 alkyl; R1 and R3 = H or (un)substituted alkyl, alkenyl, cycloalkyl, aralkyl, or aryl; R2 = H or (un)substituted alkyl; NR<sub>1</sub>R<sub>2</sub> can be a saturated 5- or 6-membered ring; R4 = (un)substituted alkyl, cycloalkyl, aralkyl, or aryl; R5 = Cl, Br, CONH<sub>2</sub>, or CN; and R6 = H, CONH<sub>2</sub>, or CN. I gave fast orange to bluish red dyeing or prints on polyester or cotton-polyester textiles. Typical dyes (all prepared by conventional diazotization and coupling of 5-aminoisothiazoles) are I (R = Me, R1 = H, R2 = C<sub>6</sub>H<sub>4</sub>OMe-*o*, R3 = cyclohexyl, R4 = Ph, R5 = R6 = CN) [96856-13-2], bluish red on cotton-polyester, and I (R = Me, R1 = R3 = H, R2 = CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>OPh, R4 = Me, R5 = R6 = CN) [96856-14-3], orange on polyester. Numerous other I are reported.

IT 96856-12-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with benzoyl chloride)

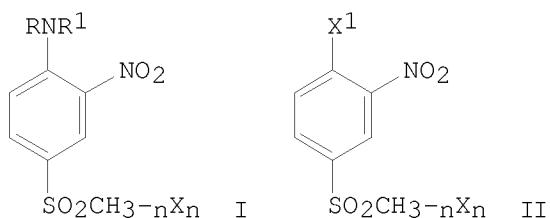
RN 96856-12-1 HCAPLUS

CN 3-Pyridinecarbonitrile, 5-[2-(4-cyano-3-phenyl-5-isothiazolyl)diazenyl]-6-[(1-(hydroxymethyl)propyl)amino]-2-[(2-methoxyphenyl)amino]-4-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

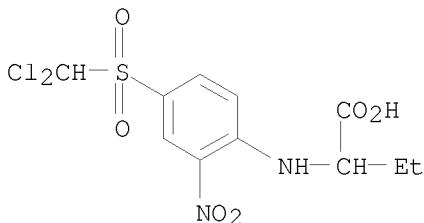
L11 ANSWER 48 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1984:630056 HCAPLUS  
 DOCUMENT NUMBER: 101:230056  
 ORIGINAL REFERENCE NO.: 101:34925a, 34928a  
 TITLE: Studies on SNAr reactions of  
 4-(halogenmethylsulfonyl)-2-nitrohalobenzene with  
 amine derivatives  
 AUTHOR(S): Ejmcocki, Zdzislaw; Eckstein, Zygmunt; Krasinski,  
 Pawel; Zagorska, Krystyna  
 CORPORATE SOURCE: Inst. Org. Chem. Technol., Polytech. Univ., Warsaw,  
 00662, Pol.  
 SOURCE: Polish Journal of Chemistry (1983), 57(4-5-6), 555-60  
 CODEN: PJCHDQ; ISSN: 0137-5083  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 101:230056  
 GI



AB Thirty-seven amino(halomethylsulfonyl)nitrobenzenes I (RR1N = NH2, Et2N,

morpholino,  $\text{CH}(\text{CHMe}_2)\text{CO}_2\text{Et}$ ,  $\text{NHCH}_2\text{CO}_2\text{Et}$ ,  $\text{PhNH}$ ,  $\text{NHCHPhCO}_2\text{Et}$ , cyclohexylamino, etc.;  $\text{X} = \text{Cl, Br}$ ;  $n = 1, 2$ ) were prepared by bimol. aromatic substitution (SNAr) reaction of the title compds. II ( $\text{X}_1 = \text{Cl, Br}$ ) with  $\text{RR}_1\text{NH}$ .

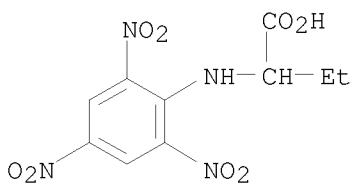
IT 61497-19-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 61497-19-6 HCPLUS  
 CN Butanoic acid, 2-[(4-[(dichloromethyl)sulfonyl]-2-nitrophenyl]amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
 (3 CITINGS)

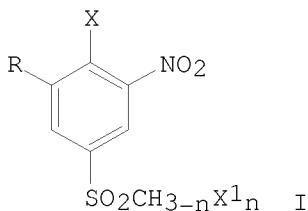
L11 ANSWER 49 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1983:64877 HCPLUS  
 DOCUMENT NUMBER: 98:64877  
 ORIGINAL REFERENCE NO.: 98:9769a,9772a  
 TITLE: Trinitrobenzenesulfonic acid: a chromophore, electrophore and precolumn derivatizing agent for high performance liquid chromatography of alkylamines  
 Caudill, W. Lowry; Wightman, R. Mark  
 AUTHOR(S):  
 CORPORATE SOURCE: Dep. Chem., Indiana Univ., Bloomington, IN, 47405, USA  
 SOURCE: Analytica Chimica Acta (1982), 141, 269-78  
 CODEN: ACACAM; ISSN: 0003-2670  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Trinitrobenzenesulfonic acid (TNBS) is an ideal precolumn derivatizing agent for high-performance liquid chromatog. of alkyl amines. The reaction is quant. and the trinitrophenyl derivs. are amenable to UV and electrochem. detection. Electrochem. detection with either a glassy C or pressure-annealed pyrolytic graphite working electrode provides lower detection limits than UV detection and thus is preferable for trace detns. The applicability of TNBS for the separation and detection of amino acids is described.

IT 84328-76-7P  
 RL: ANST (Analytical study); PREP (Preparation)  
 (preparation of)  
 RN 84328-76-7 HCPLUS  
 CN Butanoic acid, 2-[(2,4,6-trinitrophenyl)amino]- (CA INDEX NAME)



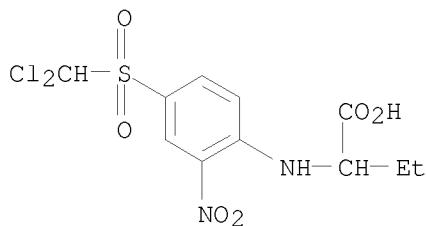
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

L11 ANSWER 50 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1977:42730 HCAPLUS  
 DOCUMENT NUMBER: 86:42730  
 ORIGINAL REFERENCE NO.: 86:6797a,6800a  
 TITLE: Use of the SNAr reaction for transformation of halonitrobenzene derivatives into biologically active agrochemicals  
 AUTHOR(S): Ejmocki, Zdzislaw  
 CORPORATE SOURCE: Inst. Chem. Technol. Org., Politech. Warsaw, Warsaw, Pol.  
 SOURCE: Prace Naukowe - Politechnika Warszawska, Chemia (1975), 17, 93 pp.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Polish  
 GI



AB Examination of the influence of  $\text{SO}_2\text{CH}_3\text{-}_n\text{X}_1\text{n}$  groups ( $\text{X}_1 = \text{Br}$  or  $\text{Cl}$ ,  $n = 0, 1$  or  $2$ ) in nucleophilic substitution reactions of halobenzenes and nitrohalobenzenes I ( $\text{R} = \text{H}$  or  $\text{NO}_2$ ;  $\text{X} = \text{Br}$ ,  $\text{Cl}$  or iodine;  $\text{X}_1 = \text{Br}$  or  $\text{Cl}$ ;  $n = 0, 1$  or  $2$ ) showed that these groups enhanced the displacement of aromatic halogen, while the halogen of the halomethyl groups resisted displacement. A substitution reaction mechanism involving a Meisenheimer  $\sigma$ -complex was suggested. All of the 150 compds. prepared were characterized and a number were found effective as fungicides and herbicides.

IT 61497-19-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 61497-19-6 HCAPLUS  
 CN Butanoic acid, 2-[(4-[(dichloromethyl)sulfonyl]-2-nitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 51 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1976:107087 HCAPLUS

DOCUMENT NUMBER: 84:107087

ORIGINAL REFERENCE NO.: 84:17455a, 17458a

TITLE: Coupling components for azo dyes

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 15

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49094677	A	19740909	JP 1972-125836	19721216
JP 52046230	B	19771122		
US 29640	E	19780523	US 1976-711863	19760805
PRIORITY APPLN. INFO.:				
		DE 1970-2062717	A	19701219
		DE 1971-2156545	A	19711115
		US 1971-209431	A2	19711217
		DE 1972-2211663	A	19720310
		DE 1972-2216570	A	19720406
		DE 1972-2226933	A	19720602
		DE 1972-2251702	A	19721021
		DE 1972-2251719	A	19721021
		DE 1972-2258823	A	19721201
		DE 1972-2259103	A	19721202
		DE 1972-2259684	A	19721206
		DE 1972-2260827	A	19721213
		GB 1972-57442	A	19721213
		JP 1972-125836	A	19721216
		DE 1972-2263458	A	19721227
		US 1973-328459	A5	19730131

GI For diagram(s), see printed CA Issue.

AB Coupling components I (R, R3 = alkyl, cycloalkyl, aryl, or O-containing aliphatic

groups; R1 = H, alkyl; R2 = CN, CONH<sub>2</sub>) for azo dyes are prepared by reaction of chloropyridine derivs. II (R<sub>4</sub> = Cl, RNH) with R<sub>3</sub>NH<sub>2</sub>. Thus, 187 parts II (R<sub>1</sub> = Me, R<sub>2</sub> = CN, R<sub>4</sub> = Cl) [875-35-4] in 500 parts MeOH was heated 5-6 hr at 40-5° with 80 parts HOCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> [141-43-5] in the presence of 100 parts Et<sub>3</sub>N, diluted with 1000 parts H<sub>2</sub>O and acidified with 50 parts concentrated HCl to give 210 parts II (R<sub>1</sub> = Me, R<sub>2</sub> = CN on left, R<sub>4</sub> = NHCH<sub>2</sub>CH<sub>2</sub>OH) [52982-62-4] containing traces of its isomer, as a colorless powder. This powder (125 parts) was stirred 6 hr with 300 parts

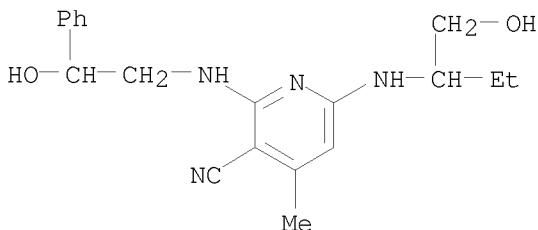
MeOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> [109-85-3] to give I (R = CH<sub>2</sub>CH<sub>2</sub>OMe, R<sub>1</sub> = Me, R<sub>2</sub> = CN, R<sub>3</sub> = CH<sub>2</sub>CH<sub>2</sub>OH) [38841-87-1] containing traces of its isomer. By similar means an addnl. 42 II (R<sub>2</sub> = Cn), 14 II (R = CONH<sub>2</sub>), 272 I (R<sub>2</sub> = CN), and 67 I (R<sub>2</sub> = CONH<sub>2</sub>) were prepared I (R = MeOCH<sub>2</sub>CH<sub>2</sub>, R<sub>1</sub> = Me, R<sub>2</sub> = CN, R<sub>3</sub> = CH<sub>2</sub>CH<sub>2</sub>Ph) [58445-83-3] was hydrolyzed with 90% H<sub>2</sub>SO<sub>4</sub> at 80-100° for 6-8 hr to give I (R, R<sub>1</sub>, R<sub>3</sub> unchanged, R<sub>2</sub> = CONH<sub>2</sub>) [52981-95-0], which coupled with diazotized p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> to give a red dye.

IT 52983-60-5P

RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of)

RN 52983-60-5 HCPLUS

CN 3-Pyridinecarbonitrile, 6-[[1-(hydroxymethyl)propyl]amino]-2-[(2-hydroxy-2-phenylethyl)amino]-4-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

L11 ANSWER 52 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1975:508362 HCPLUS

DOCUMENT NUMBER: 83:108362

ORIGINAL REFERENCE NO.: 83:16933a,16936a

TITLE: Chemotherapeutically active nitro compounds. 1.  
NitroanilinesAUTHOR(S): Winkelmann, E.; Raether, W.; Dittmar, W.; Duewel, D.;  
Gericke, D.; Hohorst, W.; Rolly, H.; Schrinner, E.

CORPORATE SOURCE: Hoechst A.-G., Frankfurt/Main, Fed. Rep. Ger.

SOURCE: Arzneimittel-Forschung (1975), 25(5), 681-708

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Of 201 nitro compds. tested, mostly basic disubstituted nitroanilines, a number were active in vitro or in vivo against bacteria, fungi, protozoa, helminths, viruses, and tumors. The activity against viruses probably resulted from increased interferon production by the host animal. The compds. with antitumor activity were effective against ascites tumors but not against solid tumors, indicating a low therapeutic index. The compds. active against protozoa and helminths also showed a low therapeutic index. Among the most active compds. were:

4-chloro-6-[(3-diethylamino-2-hydroxypropyl)amino]-1,3-dinitrobenzene [17220-91-6] and 1,2-bis(5-chloro-2,4-dinitroanilino)ethane [56225-11-7] against dermatophytes and *Candida albicans* in vitro;  
6-[(2-diethylaminoethyl)amino]-1,3-dinitro-4-methoxybenzene [17215-71-3] against *Trichomonas fetus* peritonitis in mice;  
bis[4-[(2-diethylaminoethyl)amino]-3-nitrophenyl] sulfone dihydrochloride

## STN Search

[56225-14-0] against *Entamoeba histolytica* liver necrosis in hamsters; 4-chloro-1,3-dinitro-6-(4-hydroxyphenylamino)benzene [56224-39-6] against coccidiosis in chicks; 4,6-bis[(2-dimethylaminopropyl)amino]-1,3-dinitrobenzene-2HCl (I) [17215-65-5] against *Schistosoma mansoni* in mice; 4,6-bis[(2-diethylaminoethyl)amino]-1,3-dinitrobenzene-2HCl [17215-46-2] and I against a variety of viruses in mice; and 4-chloro-1,3-dinitro-6-[4-(2-hydroxyethyl)piperazino]benzene [56224-38-5] against Ehrlich carcinoma in mice.

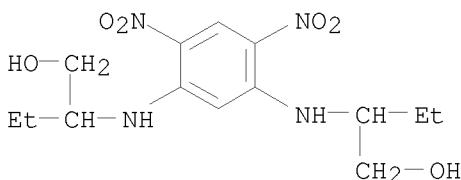
IT 56224-49-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and anthelmintic and antimicrobial and antitumor activity of)

RN 56224-49-8 HCAPLUS

CN 1-Butanol, 2,2'-(4,6-dinitro-1,3-phenylene)diimino]bis- (9CI) (CA INDEX NAME)



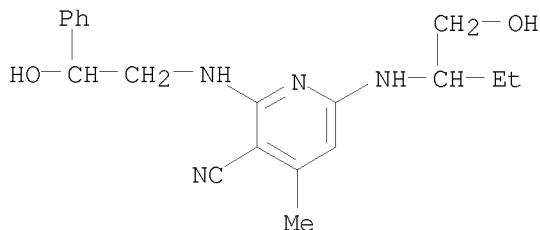
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
(4 CITINGS)

L11 ANSWER 53 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1975:461736 HCAPLUS  
DOCUMENT NUMBER: 83:61736  
ORIGINAL REFERENCE NO.: 83:9757a, 9760a  
TITLE: Coupling components for azo dyes  
INVENTOR(S): Dehnert, Johannes; Lamm, Gunther  
PATENT ASSIGNEE(S): BASF A.-G.  
SOURCE: Ger. Offen., 56 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 15  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2260827	A1	19740711	DE 1972-2260827	19721213
DE 2260827	B2	19800320		
DE 2260827	C3	19801113		
US 29640	E	19780523	US 1976-711863	19760805
PRIORITY APPLN. INFO.:			DE 1970-2062717	A 19701219
			DE 1971-2156545	A 19711115
			US 1971-209431	A2 19711217
			DE 1972-2211663	A 19720310
			DE 1972-2216570	A 19720406
			DE 1972-2226933	A 19720602
			DE 1972-2251702	A 19721021

DE	1972-2251719	A	19721021
DE	1972-2258823	A	19721201
DE	1972-2259103	A	19721202
DE	1972-2259684	A	19721206
DE	1972-2260827	A	19721213
GB	1972-57442	A	19721213
JP	1972-125836	A	19721216
DE	1972-2263458	A	19721227
US	1973-328459	A5	19730131

GI For diagram(s), see printed CA Issue.  
 AB Azo coupler (I, R = CN, CONH<sub>2</sub>; R<sub>1</sub> = H, alkyl, substituted alkyl, cycloalkyl; R<sub>2</sub> = H, alkyl, substituted alkyl, Ph, substituted Ph, cycloalkyl) were prepared. Thus, 2,6-dichloro-3-cyano-4-methylpyridine was suspended in MeOH and heated with HOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> in the presence of Et<sub>3</sub>N at 45-50° for 5-6 hr to give a mixture consisting predominantly of 6-chloro-3-cyano-2-[(2-hydroxyethyl)amino]-4-methylpyridine which was refluxed with MeOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> to give a mixture predominantly of pyridine coupler (I, R = CN, R<sub>1</sub> = MeOCH<sub>2</sub>CH<sub>2</sub>, R<sub>2</sub> = HOCH<sub>2</sub>CH<sub>2</sub>). The other I were similarly prepared  
 IT 52983-60-5P  
 RL: IMF (Industrial manufacture); PREP (Preparation)  
 (preparation of)  
 RN 52983-60-5 HCPLUS  
 CN 3-Pyridinecarbonitrile, 6-[[1-(hydroxymethyl)propyl]amino]-2-[(2-hydroxy-2-phenylethyl)amino]-4-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)

L11 ANSWER 54 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1975:444734 HCPLUS  
 DOCUMENT NUMBER: 83:44734  
 ORIGINAL REFERENCE NO.: 83:7095a,7098a  
 TITLE: Substituted 2,6-diamino-4-methylnicotinonitriles, the corresponding nicotinamides and derivatives  
 INVENTOR(S): Lamm, Gunther; Dehnert, Johannes  
 PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.  
 SOURCE: U.S., 19 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 15  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3853895	A 19741210	US 1973-328459	19730131
US 29640	E 19780523	US 1976-711863	19760805
PRIORITY APPLN. INFO.:			
		DE 1970-2062717	A 19701219
		DE 1971-2156545	A 19711115
		US 1971-209431	A2 19711217
		DE 1972-2211663	A 19720310
		DE 1972-2216570	A 19720406
		DE 1972-2226933	A 19720602
		DE 1972-2251702	A 19721021
		DE 1972-2251719	A 19721021
		DE 1972-2258823	A 19721201
		DE 1972-2259103	A 19721202
		DE 1972-2259684	A 19721206
		DE 1972-2260827	A 19721213
		GB 1972-57442	A 19721213
		JP 1972-125836	A 19721216
		DE 1972-2263458	A 19721227
		US 1973-328459	A5 19730131

GI For diagram(s), see printed CA Issue.

AB Diaminopyridine couplers (I, R, R2 = H, alkyl, substituted alkyl, Ph, substituted Ph, cycloalkyl, norbornyl, arylalkyl, R1 = CN, CONH2) were prepared and were useful for preparation of azo dyes by coupling with diazotized

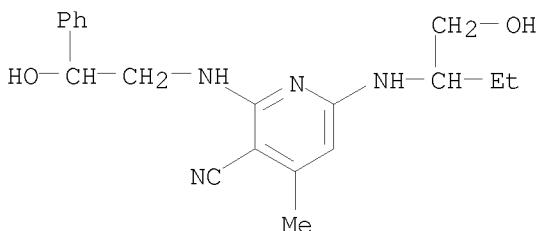
amines. Thus, 2,6-dichloro-3-cyano-4-methylpyridine [875-35-4] was suspended in MeOH, HOCH2CH2NH2 [141-43-5] was added, the mixture stirred at 45-50° for 5-6 hr to give predominantly 6-chloro-3-cyano-2-[(2-hydroxyethyl)amino]-4-methylpyridine [52982-62-4] which was refluxed in MeOCH2CH2NH2 [109-85-3] to give coupler I(R = MeOCH2CH2, R1 = CN, R2 = HOCH2CH2) [55635-93-3]. The other 200 I were similarly prepared

IT 52983-60-5P

RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of)

RN 52983-60-5 HCPLUS

CN 3-Pyridinecarbonitrile, 6-[[1-(hydroxymethyl)propyl]amino]-2-[(2-hydroxy-2-phenylethyl)amino]-4-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
(8 CITINGS)

L11 ANSWER 55 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

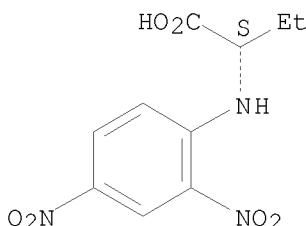
ACCESSION NUMBER: 1974:96332 HCPLUS

DOCUMENT NUMBER: 80:96332

ORIGINAL REFERENCE NO.: 80:15507a,15510a

TITLE: Partial asymmetric syntheses of amino acids using lithium aldimine precursors  
 AUTHOR(S): Hirowatari, N.; Walborsky, H. M.  
 CORPORATE SOURCE: Dep. Chem., Florida State Univ., Tallahassee, FL, USA  
 SOURCE: Journal of Organic Chemistry (1974), 39(5), 604-7  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Carboxylation or carbethoxylation of Li aldimines PhCMeEtN:CRLi (R = MeCHEt, Et, CHMe<sub>2</sub>) formed by the  $\alpha$  addition of EtLi, MeCHEtLi, or Me<sub>2</sub>CHLi to ( $\pm$ )- or (R)-(+)-PhCMeEtNC gave the corresponding  $\alpha$ -imino acids or esters which were reduced to the  $\alpha$ -amino acids.  
 IT 4470-69-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 4470-69-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
 (5 CITINGS)

L11 ANSWER 56 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1973:97984 HCPLUS  
 DOCUMENT NUMBER: 78:97984  
 ORIGINAL REFERENCE NO.: 78:15735a,15738a  
 TITLE: Sterically controlled syntheses of optically active organic compounds. XVIII. Asymmetric syntheses of optically active amino acids by addition of hydrogen cyanide to Schiff bases  
 AUTHOR(S): Harada, Kaoru; Okawara, Tadashi  
 CORPORATE SOURCE: Inst. Mol. Cell. Evol., Univ. Miami, Coral Gables, FL, USA  
 SOURCE: Journal of Organic Chemistry (1973), 38(4), 707-10  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Addition reactions of HCN to Schiff bases which were prepared from several aliphatic aldehydes and optically active benzylic amines were studied. The addition products were hydrolyzed and hydrogenolyzed to form optically active amino acids. The synthetic yields of amino acids were in a range of 9-58% and the optical purities of amino acids without fractionation of optical isomers were in a range of 22-58%. When (R)- $\alpha$ -alkylbenzylamines were used, (R)-amino acids were obtained.

The fractionation of optical isomers during isolation and purification was examined

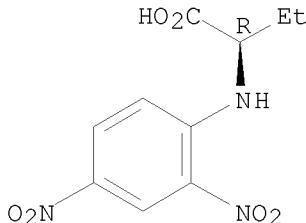
IT 6367-34-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 6367-34-6 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

L11 ANSWER 57 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1973:97981 HCPLUS

DOCUMENT NUMBER: 78:97981

ORIGINAL REFERENCE NO.: 78:15735a,15738a

TITLE: Sterically controlled synthesis of optically active organic compounds. XVII. Asymmetric syntheses of amino acids by addition of benzoyl cyanide to the azomethine compounds

AUTHOR(S): Harada, Kaoru; Okawara, Tadashi

CORPORATE SOURCE: Inst. Mol. Cell. Evol., Univ. Miami, Coral Gables, FL, USA

SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(1), 191-3

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

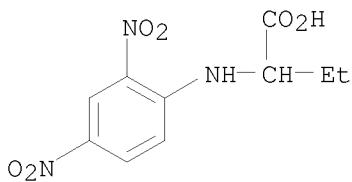
AB The addition reactions of  $\text{PhCOCN}$  with Schiff's bases prepared from aliphatic aldehydes and optically active benzylic amines were studied. The addition products were hydrolyzed and hydrogenolyzed to optically active amino acids in yields of 15-57% with optical purities of 15-37%. When  $\text{S-}\alpha\text{-alkylbenzylamines}$  were used,  $\text{S-amino acids}$  were obtained.

IT 31356-29-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

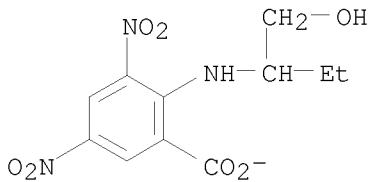
RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 58 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1971:448107 HCPLUS  
 DOCUMENT NUMBER: 75:48107  
 ORIGINAL REFERENCE NO.: 75:7585a, 7588a  
 TITLE: Steric acceleration of a ring closure to an oxazepinone by steric hindrance  
 AUTHOR(S): Turk, Jonathan; Haney, William M.; Heid, Georgia; Barlow, Richard E.; Clapp, Leallyn B.  
 CORPORATE SOURCE: Dep. Chem., Brown Univ., Providence, RI, USA  
 SOURCE: Journal of Heterocyclic Chemistry (1971), 8(1), 149-51  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB The gem-dialkyl substitution of benzoic acids, 2,4,6-HOCH<sub>2</sub>CRR<sub>1</sub>NH(O<sub>2</sub>N)C<sub>6</sub>H<sub>2</sub>CO<sub>2</sub>H, accelerates closure to the corresponding 1,2,3,5-tetrahydro-5-oxo-4,1-benzoxazepines (I). 5-Nitro-1-(2-hydroxyethyl)benzotriazole-7-carboxylic acids (II) in the same manner. 9-Nitro-7-oxo-*v*-triazolo[4,5,1-*jk*][4,1]benzoxazepines (III) are prepared. The acceleration is greater in the case of II.  
 IT 33414-90-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 33414-90-3 HCPLUS  
 CN Benzenemethanaminium, N,N,N-trimethyl-, 2-[1-(hydroxymethyl)propyl]amino]-3,5-dinitrobenzoate (1:1) (CA INDEX NAME)  
 CM 1  
 CRN 47141-03-7  
 CMF C11 H12 N3 O7



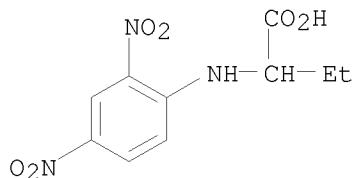
CM 2

CRN 14800-24-9  
CMF C10 H16 N

Me<sub>3</sub><sup>+</sup>N—CH<sub>2</sub>—Ph

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 59 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1971:60669 HCAPLUS  
DOCUMENT NUMBER: 74:60669  
ORIGINAL REFERENCE NO.: 74:9753a,9756a  
TITLE: Chromatography of dinitrophenylamino acids and heterocyclic bases on thin layers of protein  
Brady, P. R.; Hoskinson, R. M.  
AUTHOR(S):  
CORPORATE SOURCE: Div. Text. Ind., C.S.I.R.O., Belmont, Australia  
SOURCE: Journal of Chromatography (1971), 54(1), 65-70  
CODEN: JOCRAM; ISSN: 0021-9673  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Rf values are given for 24 dinitrophenyl (DNP) amino acid derivs. on unmodified and esterified keratin thin layers (P. R. Brady and R. M. Hoskinson, 1971) and for 12 pyrimidines and 7 purines on the esterified keratin layers. Two-dimensional development with 3:2:1 BuOH-H<sub>2</sub>O-HOAc and 5:1 tert-amyl alc.-0.88 NH<sub>3</sub> separated 14 DNP amino acids on the unmodified keratin layers.  
IT 31356-29-3  
RL: ANT (Analyte); ANST (Analytical study)  
(chromatog. of)  
RN 31356-29-3 HCAPLUS  
CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 60 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1970:505492 HCAPLUS  
DOCUMENT NUMBER: 73:105492  
ORIGINAL REFERENCE NO.: 73:17167a,17170a  
TITLE: Mass spectrometry of DNP [2,4-dinitrophenyl]-amino acids combination with paper chromatography  
Studier, Martin H.; Moore, Leon P.; Hayatsu, Ryoichi;  
Matsuoka, Sumiko  
AUTHOR(S):  
CORPORATE SOURCE: Chem. Div., Argonne Nat. Lab., Argonne, IL, USA  
SOURCE: Biochemical and Biophysical Research Communications  
(1970), 40(4), 894-900  
CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The DNP derivs. of 20 amino acids were prepared and their mass spectra determined

The anal. application of the combination of mass spectrometry and paper chromatog. was demonstrated.

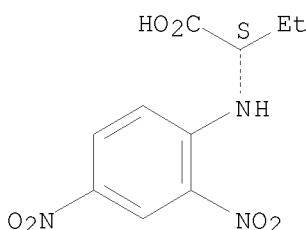
IT 4470-69-3

RL: PRP (Properties)  
(mass spectrum of)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

L11 ANSWER 61 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1970:121890 HCPLUS

DOCUMENT NUMBER: 72:121890

ORIGINAL REFERENCE NO.: 72:21943a,21946a

TITLE: Sterically controlled syntheses of optically active compounds. IX. Syntheses of optically active amino acids by reduction of Schiff bases with sodium borohydride

AUTHOR(S): Harada, Kaoru; Ohhashi, Junichi

CORPORATE SOURCE: Inst. of Mol. Evol., Univ. of Miami, Coral Gables, FL, USA

SOURCE: Bulletin of the Chemical Society of Japan (1970), 43(3), 960-3  
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The Schiff bases of  $\alpha$ -oxo acids with optically active  $\alpha$ -alkylbenzylamines were reduced with NaBH4, and the reduced compds. were hydrogenolyzed and hydrolyzed to give  $\alpha$ -amino acids, which were converted to their corresponding DNP-amino acids by treatment with 2,4-dinitrofluorobenzene. The yields of the asym. synthesis and the optical purity of synthesized amino acids were rather low.

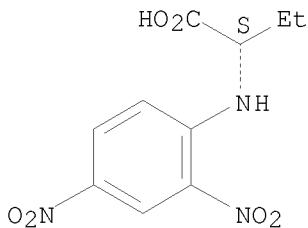
IT 4470-69-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 62 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1970:32100 HCPLUS

DOCUMENT NUMBER: 72:32100

ORIGINAL REFERENCE NO.: 72:5901a,5904a

TITLE: Absolute configurations of the alkaloids of *Physostigma venenosum* seeds

AUTHOR(S): Longmore, R. B.; Robinson, Brian

CORPORATE SOURCE: Dep. Pharm., Univ. Manchester, Manchester, UK

SOURCE: Journal of Pharmacy and Pharmacology (1969), 21(Suppl.), 118-25

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: English

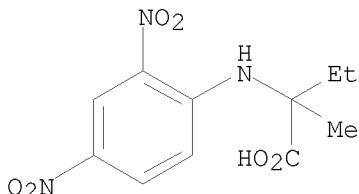
AB The absolute configuration of physostigmine was established by correlating the configuration of its C-3a atom with that of the asymmetric C atom in (+)-3-ethyl-3-methoxycarbonyl-3-methylpropionic acid. Comparison of the ORD spectra of physostigmine, Na-norphysostigmine, geneserine, physovenine and eseramine have shown that all five alkaloids have the same absolute configurations.

IT 25471-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 25471-53-8 HCPLUS

CN Isovaline, N-(2,4-dinitrophenyl)-, (DL)- (8CI) (CA INDEX NAME)



L11 ANSWER 63 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1967:464664 HCPLUS

DOCUMENT NUMBER: 67:64664

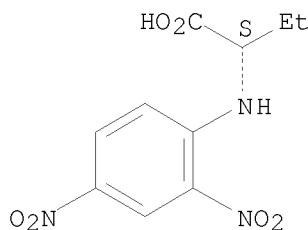
ORIGINAL REFERENCE NO.: 67:12207a,12210a

TITLE: Synthesis of optically active  $\alpha$ -amino-acids from  $\alpha$ -oxo acids by hydrogenolytic asymmetric transamination

AUTHOR(S): Harada, Kaoru

CORPORATE SOURCE: Univ. of Miami, Coral Gables, FL, USA  
 SOURCE: Nature (London, United Kingdom) (1966), 212(5070),  
 1571-2  
 CODEN: NATUAS; ISSN: 0028-0836  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB MeCH<sub>2</sub>COCO<sub>2</sub>H (1.02 g.) and 1.51 g. L-phenylglycine, [α]25D  
 168° (5N HCl), were dissolved in a mixture of 10.0 ml. 2N NaOH and 10  
 ml. H<sub>2</sub>O. After standing 30 min. at room temperature, the solution was  
 hydrogenated  
 and hydrogenolyzed with 2.50 g. 10% Pd/C (initial pressure 40 lb.). After  
 24 hrs. of reaction, the catalyst was removed by filtration. The catalyst  
 was washed repeatedly with H<sub>2</sub>O. The filtrate was concentrated, to .apprx.25  
 ml.  
 and 6N HCl was added to bring the pH to .apprx.1. The precipitated PhCH<sub>2</sub>CO<sub>2</sub>H  
 was  
 extracted with ether. The aqueous solution was evaporated to dryness. The  
 amino  
 acid-HCl was extracted with absolute alc. and the insol. NaCl filtered off.  
 The  
 alc. solution was evaporated to dryness and the remaining amino acid-HCl  
 dissolved in 15 ml. H<sub>2</sub>O. The aqueous solution was applied to a Dowex column (H  
 form, 100-200 mesh, 2 cm. + 13 cm.). MeCH<sub>2</sub>CH(OH)CO<sub>2</sub>H and other  
 non-amino acid acidic materials were eluted with H<sub>2</sub>O, and MeCH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H  
 was then eluted with N aqueous NH<sub>3</sub> to give 0.36 g. precipitate, [α]25D  
 7.3°.  
 IT 4470-69-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 4470-69-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
 (3 CITINGS)

L11 ANSWER 64 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1967:422127 HCPLUS  
 DOCUMENT NUMBER: 67:22127  
 ORIGINAL REFERENCE NO.: 67:4243a  
 TITLE: Sterically controlled synthesis of optically active  
 organic compounds. V. Sterically controlled  
 synthesis of optically active α-amino acids from  
 α-oxo acids by reductive amination  
 AUTHOR(S): Harada, Kaoru; Matsumoto, Kazuo

CORPORATE SOURCE: Univ. of Miami, Coral Gables, FL, USA  
 SOURCE: Journal of Organic Chemistry (1967), 32(6), 1794-800  
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal  
 LANGUAGE: English

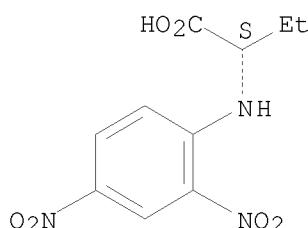
AB To clarify the steric courses of the asym. syntheses of  $\alpha$ -amino acids from  $\alpha$ -oxo acids with optically active amines, 3 kinds of reactions were carried out: (A) hydrogenation of the Schiff bases of  $\alpha$ -oxo acids with (R,S)- $\alpha$ -methylbenzylamine and with (R,S)- $\alpha$ -ethylbenzylamine; (B) (1) hydrogenation of oximes of N-(R,S)- $\alpha$ -methylbenzylbenzoyl-formamide and of N-(R,S)- $\alpha$ -ethylbenzylbenzoylformamide; (2) hydrogenation of benzylamine Schiff bases of pyruvyl-(S)-alanine iso-Bu ester and of pyruvyl-(R)-and-(S)-valine iso-Bu ester; (C) hydrogenation of the Schiff bases of 1-methyl pyruvate with (R,S)- $\alpha$ -methylbenzylamine and with (R,S)- $\alpha$ -ethylbenzylamine. In each reaction, possible steric courses are discussed. 26 references.

IT 4470-69-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L11 ANSWER 65 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1967:422126 HCPLUS  
 DOCUMENT NUMBER: 67:22126  
 ORIGINAL REFERENCE NO.: 67:4242h, 4243a  
 TITLE: Sterically controlled syntheses of optically active organic compounds. IV. Syntheses of optically active  $\alpha$ -amino acids from  $\alpha$ -oxo acids by hydrogenolytic asymmetric transamination  
 AUTHOR(S): Harada, Kaoru  
 CORPORATE SOURCE: Univ. of Miami, Coral Gables, FL, USA  
 SOURCE: Journal of Organic Chemistry (1967), 32(6), 1790-3  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB cf. CA 65: 3956c, 13816b. Na  $\alpha$ -phenylglycinate was found to be hydrogenolyzed easily to NH<sub>3</sub> and phenylacetic acid using Pd as the catalyst. By the use of this result, asym. syntheses of  $\alpha$ -amino acids from their corresponding  $\alpha$ -oxo acids with optically active

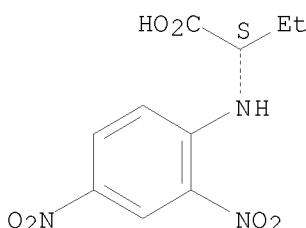
$\alpha$ -phenylglycine in aqueous alkaline solution were investigated. Optically active alanine,  $\alpha$ -aminobutyric acid, glutamic acid, and aspartic acid were synthesized. Optical purities of these synthesized amino acids were in the range of 40 to 60%.

IT 4470-69-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 4470-69-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 66 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1967:16957 HCPLUS

DOCUMENT NUMBER: 66:16957

ORIGINAL REFERENCE NO.: 66:3255a,3258a

TITLE: Gas chromatographic separation of dinotrophenyl amino acids and its application to the analysis of serum amino acids

AUTHOR(S): Ikekawa, Nobuo; Hoshino, Osamu; Watanuki, Reiko

CORPORATE SOURCE: Inst. Phys. Chem. Res., Tokyo, Japan

SOURCE: Analytical Biochemistry (1966), 17(1), 16-23

CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for the separation and estimation of dinitrophenyl (DNP) derivs. of 13 amino acids by a gas chromatographic technique is described. The separation was carried out with 1.0% XE-61 or 1.5% SE-30 as the stationary phase, and with a H flame ionization detector and temperature programmer. A method for

the

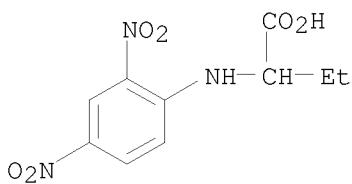
determination of the free amino acids in serum by gas chromatography was also investigated. 17 references.

IT 31356-29-3

RL: ANT (Analyte); ANST (Analytical study)  
(chromatog. of)

RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 67 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1966:421096 HCPLUS

DOCUMENT NUMBER: 65:21096

ORIGINAL REFERENCE NO.: 65:3956d-h, 3957a

TITLE: Synthesis of tripeptides of serine and lysine with different sequences of the amino acids

AUTHOR(S): El Naggar, Ahmed M.; Poddubnaya, N. A.

SOURCE: Sintez Prirod. Soedin., ikh Analogov i Fragmentov, Akad. Nauk SSSR, Otd. Obshch. i Tekhn. Khim. (1965) 179-83

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB In order to study the fragments obtained from peptide antibiotics, the synthesis of di- and tripeptides containing lysine and serine is described. Dipeptides are prepared by reaction of formyl and carbobenzoxy (Cbz) derivs. of one amino acid with the Me ester of the other in the presence of dicyclohexylcarbodiimide. The resulting dipeptide ester is converted by reaction with N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O to the hydrazide which is then treated with NaNO<sub>2</sub> in an acid to obtain the azide. Reaction of the azide with an amino acid esters gives the tripeptide derivative To a solution of 2 g.

Na-Cbz-DL-serine, 2.8 g. Me ester of Nε-Cbz-DL-lysine-HCl, and 1.2 ml. absolute Me<sub>3</sub>N in 40 ml. absolute MeNO<sub>2</sub> was added 2 g. dicyclohexylcarbodiimide. The solution was heated 30 min. to 40° and then allowed to stand overnight. After removing the precipitated dicyclohexylurea by filtration, the filtrate was evaporated in vacuo. The oily residue was dissolved in EtOAc and Me<sub>3</sub>N.HCl filtered off. The residue after evaporation of the filtrate was crystallized from absolute Et<sub>2</sub>O to give

4.2 g. Me ester of N-Cbz-DL-seryl-Nε-Cbz-DL-lysine (I), m.

150-2°. Similarly prepared were the Me esters of

Na-formyl-Nε-Cbz-DL-lysyl-Nε-Cbz-DL-lysine (m.

75-8°, yield 87%), and Na-formyl-Nε-Cbz-DL-lysyl-DL-

serine, m. 118-20°, yield 59%.

Na-formyl-Nε-Cbz-DL-lysine was prepared from

Nε-Cbz-DL-lysine by treatment with 100% HCO<sub>2</sub>H and Ac<sub>2</sub>O. To a solution of 2 g. I in 35 ml. absolute hot MeOH was added 1.02 ml. N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O and the mixture allowed to stand 48 hrs. at room temperature. The 1.2 g. of the N-Cbz-DL-seryl-Nε-Cbz-DL-lysine hydrazide (II) (m. 165-8°), which precipitated, plus 0.5 g. obtained by concentration of the mother liquor

gave a

total yield of 1.7 g. Similarly prepared were

Na-formyl-Nε-Cbz-DL-lysyl-Nε-Cbz-DL-lysine

hydrazide, m. 162-3°, yield 88%, and

Na-formyl-Nε-Cbz-DL-lysyl-DL-serine hydrazide, m.

184-6°, yield 88%. To a cold (-5° to -10°) solution of

1 g. II in 40 ml. H<sub>2</sub>O, 3 ml. AcOH, and 1 ml. concentrated HCl, was added a cold solution of 0.3 g. NaNO<sub>2</sub> in 5 ml. H<sub>2</sub>O. The resulting mixture was stirred 5

min. and the azide extracted with 35 ml. cold EtOAc. The EtOAc extract was washed quickly with ice water, 3% aqueous NaHCO<sub>3</sub> at 0°, and twice again with ice water. The extract was dried 20 min. over Na<sub>2</sub>SO<sub>4</sub> in the cold. A solution of Me ester of serine was freshly prepared from 0.5 g. of its HCl salt in 10 ml. absolute CHCl<sub>3</sub> by addition of 0.35 ml. absolute Me<sub>3</sub>N and stirring 25 min.

Addition of absolute Et<sub>2</sub>O precipitated Me<sub>3</sub>N.HCl which was filtered off. The residue

from the filtrate after evaporation of the solvent in vacuo was dissolved in 15 ml. absolute EtOAc and cooled to 0°. To this cold solution of the ester was added the solution of the azide. After standing at room temperature 24 hrs.,

the mixture was washed twice with 0.5N HCl, twice with 3% aqueous NaHCO<sub>3</sub>, and with water. After removal of the solvent the residue was crystallized by trituration with petroleum ether to give 0.8 g. Me ester of

N-Cbz-DL-seryl-Nε-Cbz-DL-lysyl-DL-serine, m. 89-90°.

Similarly prepared were (m.p. and % yield given): Me esters of Na-formyl-Nε-Cbz-DL-lysyl-Nε-Cbz-DL-lysyl-Nε-

Cbz-DL-lysine, 112-14°, 60;

Na-formyl-Nε-Cbz-DL-lysyl-DL-seryl-DL-serine, 100-1°,

40; N-Cbz-DL-seryl-DL-seryl-Nε-Cbz-DL-lysine, 90-2°, 72;

N-Cbz-DL-seryl-Nε-Cbz-DL-lysyl-Nε-Cbz-DL-lysine,

101-2°, 85; and Na-formyl-Nε-Cbz-DL-lysyl-DL-seryl-

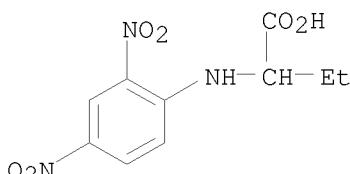
Nε-Cbz-DL-lysine, 99-100°, 56

IT 31356-29-3

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 68 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1966:421095 HCPLUS

DOCUMENT NUMBER: 65:21095

ORIGINAL REFERENCE NO.: 65:3956c-d

TITLE: Stereoselective syntheses of optically active amino acids from menthyl esters of  $\alpha$ -oxo acids

AUTHOR(S): Matsumoto, Kazuo; Harada, Kaoru

CORPORATE SOURCE: Univ. of Miami, Coral Gables, FL

SOURCE: Journal of Organic Chemistry (1966), 31(6), 1956-8

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 65:21095

AB Menthyl esters of pyruvic acid,  $\alpha$ -oxobutyric acid, and phenylglyoxylic acid were converted to their oximes and Schiff bases of benzylamine. These were hydrogenated catalytically by the use of Pd-C and palladium hydroxide on charcoal. Optically active D-alanine (optical

yield 16-25%), D- $\alpha$ -aminobutyric acid (8-21%), and D-phenyl-glycine (44-49%) were obtained. Possible steric courses of the reactions are discussed.

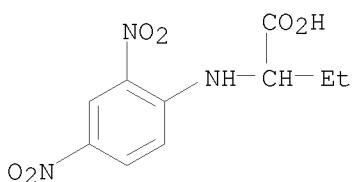
IT 31356-29-3

RL: PREP (Preparation)

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L11 ANSWER 69 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1965:489203 HCAPLUS

DOCUMENT NUMBER: 63:89203

ORIGINAL REFERENCE NO.: 63:16440g-h

TITLE: Amino derivatives of starches. Derivatives of 3,6-diamino-3,6-dideoxy-D-altrose

AUTHOR(S): Wolfrom, M. L.; Hung, Yen-Lung; Horton, Derek

CORPORATE SOURCE: Ohio State Univ., Columbus

SOURCE: Journal of Organic Chemistry (1965), 30(10), 3394-400

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 63:89203

AB Hydrazinolysis of methyl 2,6-di-O-(methylsulfonyl)- $\alpha$ -D-glucopyranoside, followed by reduction, gives methyl 3,6-diamino-3,6-dideoxy- $\alpha$ -D-altropyranoside, isolable in high yield as the N,N'-diacetyl or N,N'-(2,4-dinitrophenyl) derivatives. The structure and stereochemistry of the product were proved by a sequence of degradation reactions and by comparison of the products with derivatives of known  $\alpha$ -amino acids. 3,6-Diacetamido-3,6-dideoxy-D-altrose was prepared by way of 3,5-diacetamido-3,6-dideoxy-D-altrose diethyl dithioacetal.

IT 4470-69-3

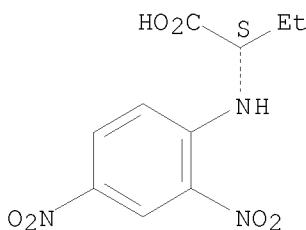
RL: PREP (Preparation)

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 4470-69-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

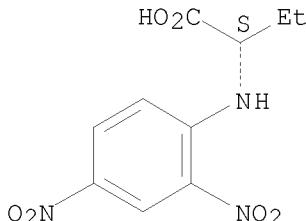
Absolute stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

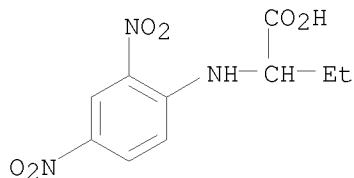
L11 ANSWER 70 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1965:489202 HCPLUS  
 DOCUMENT NUMBER: 63:89202  
 ORIGINAL REFERENCE NO.: 63:16440f-g  
 TITLE: The acid hydrolysis of laminaran  
 AUTHOR(S): Szejtli, Jozsef  
 CORPORATE SOURCE: Tech. Univ. Norway, Trondheim  
 SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1965), 45(2), 141-51  
 CODEN: ACASA2; ISSN: 0001-5407  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Laminaran was used to investigate the hydrolysis of  $\beta$ -D-(1  $\rightarrow$  3)-glucose linkages catalyzed by hydrogen ion. The rate constant of hydrolysis was determined at three different temperatures and three different concentrations of hydrochloric acid. For the equation,  $K = [aH^+]^{1/2}e^{2.303e-E_a/RT}$ ,  $g$  was found to have a value of 1.05941  $E_a$  is 31,175 cal./mol. and  $d$  is 17.108. The entropy of activation is 9.19 cal./mol.  
 IT 4470-69-3  
 RL: PREP (Preparation)  
 (Derived from data in the 7th Collective Formula Index (1962-1966))  
 RN 4470-69-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

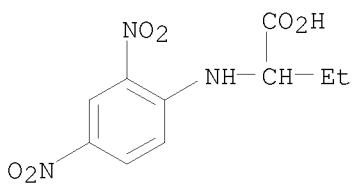


L11 ANSWER 71 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1965:442770 HCPLUS  
 DOCUMENT NUMBER: 63:42770  
 ORIGINAL REFERENCE NO.: 63:7680a-b  
 TITLE: Separation of 2,4-dinitrophenol derivatives of amino acids by high-voltage paper electrophoresis

AUTHOR(S): Fittkau, Siegfried  
 CORPORATE SOURCE: Martin-Luther Univ., Halle/Saale, Germany  
 SOURCE: Journal of Chromatography (1965), 18(2), 331-5  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB The electrophoretic mobilities of 31 2,4-dinitrophenol derivs. of amino acids, in pyridine acetate and acetateformate buffers of pH 1.8 to 6.5, at a potential of 67 v./cm., are given. Solns. in the 2 solvents were of approx. the same conductivity and the expts. were conducted with the apparatus described by the author (CA 60, 6493c) on 30 cm. wide + 60 cm. long, Schleicher and Schuell 2043a filter paper, soaked in the buffer and pressed to contain 120% of the dry paper weight. The solns. (5  $\mu$ l. of 0.02M in Me<sub>2</sub>CO or dimethylformamide) were applied 12 cm. from the cathode side of the paper's edge and a potential of 4000 v. was applied for 120 min.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)- (electrophoresis of)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)

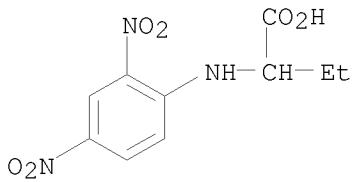


L11 ANSWER 72 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1965:442769 HCAPLUS  
 DOCUMENT NUMBER: 63:42769  
 ORIGINAL REFERENCE NO.: 63:7679h, 7680a  
 TITLE: Thin-film electrophoresis. II. Freeze-drying of electropherograms  
 AUTHOR(S): Criddle, W. J.; Moody, G. J.; Thomas, J. D. R.  
 CORPORATE SOURCE: Welsh Coll. Advanced Technol., Cardiff  
 SOURCE: Journal of Chromatography (1965), 18(3), 530-4  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB cf. CA 62, 5796h. The zone migration that occurs during the drying stage of electropherograms can be prevented by freeze-drying instead of drying at elevated temps.  
 IT 31356-29-3  
     (Derived from data in the 7th Collective Formula Index (1962-1966))  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 73 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1964:18163 HCPLUS  
 DOCUMENT NUMBER: 60:18163  
 ORIGINAL REFERENCE NO.: 60:3256g-h  
 TITLE: An improved method of separating amino acids as  
 N-2,4-dinitrophenyl derivatives  
 AUTHOR(S): Matheson, N. A.  
 CORPORATE SOURCE: Rowett Res. Inst., Aberdeen, UK  
 SOURCE: Biochemical Journal (1963), 88(1), 146-51  
 CODEN: BIJOAK; ISSN: 0264-6021  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB An improved method of separating ether-soluble dinitrophenol-(DNP)-amino acids  
 by  
 partition chromatography on short kieselguhr columns is described.  
 DNP-amino acids are partitioned, largely as ions, between aqueous buffers and  
 EtOAc; they form unusually narrow bands with a wide range of R values  
 which are much less dependent on pH than in purely nonionic partition.  
 Columns of this type allow the isolation of almost any one of the common  
 ether-soluble DNP-amino acids from a dinitrophenylated mixture within an hr.  
 or two. The R values of many of the common DNP-amino acids on columns at  
 different pH values are listed.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)-  
 (chromatography of)  
 RN 31356-29-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)

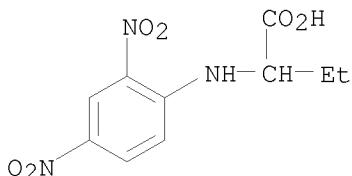


L11 ANSWER 74 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1964:18162 HCPLUS  
 DOCUMENT NUMBER: 60:18162  
 ORIGINAL REFERENCE NO.: 60:3256e-g  
 TITLE: The determination of catechol amines in biological  
 materials  
 AUTHOR(S): Callingham, B. A.; Cass, Rosemary  
 CORPORATE SOURCE: Univ. London

SOURCE: West-European Symp. Clin. Chem. (1963), 2, 19-30  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Biol. and biochem. methods for the determination of catechol amines are evaluated.

Biol. methods are now being replaced by chemical methods of high sensitivity and specificity. The choice of the various 2-step methods for purification depend largely upon the original solvent used and the tissue to be assayed. For the extraction and purification of the catechol amines in urine and blood plasma, adsorption and ion-exchange techniques are used. A strong cation-exchange resin, Dowex 50, is probably the best available method for the separation of dopamine from adrenaline and noradrenaline. Although many colorimetric methods are available for assay of catechol amines much value today is placed on paper chromatography. To obtain sensitivity with specificity, fluorimetric methods of assay are necessary. The 2 main methods utilizing fluorescence for the assay of catechol amines are the trihydroxyindole method and the ethylenediamine condensation method. The latter probably is more sensitive, and when combined with suitable ionexchange columns, may be made very specific. The chemical assay of dopamine is also discussed.

IT 31356-29-3  
 (Derived from data in the 7th Collective Formula Index (1962-1966))  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 75 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1964:18161 HCAPLUS  
 DOCUMENT NUMBER: 60:18161  
 ORIGINAL REFERENCE NO.: 60:3256b-e  
 TITLE: A simple method for the determination of urinary testosterone excretion in human urine  
 AUTHOR(S): Vermeulen, A.; Verplancke, Joseph C. M.  
 CORPORATE SOURCE: Akad. Ziekenhuis, Ghent, Belg.  
 SOURCE: Steroids (1963), 2(4), 453-63  
 CODEN: STEDAM; ISSN: 0039-128X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB A method for estimation of the title compound (I) is described which involves isotope dilution and double thin-layer chromatography in order to provide a more reliable parameter of androgen production. Thus 104 counts/min. of I-4-14C was added to half of a 24-hr. urine sample, the pH adjusted to 5.0 by addition of 0.1 volume 0.1 M acetate buffer (pH 5.4), 1000 units  $\beta$ -glucuronidase added per ml. urine, the mixture incubated 48 hrs. at 37°, and extracted 4 times with Et2O. The combined Et2O exts. were washed twice with 10% aqueous NaOH and twice with H2O, dried, and evaporated in vacuo. The residue was chromatographed on 2 g. Al2O3, elution of which

with 60 ml. 0.25% EtOH-C6H6 yielded I and 11-deoxy-17-ketosteroids. This mixture was separated by thin-layer chromatography, using CHCl3-AcOEt (80:20). The I zone was identified by ultraviolet light and eluted with Et2O, which extract was evaporated to dryness. A mixture of the residue and 0.3 ml. AcOH containing 0.2 ml. 2% CrO3 was kept overnight at room temperature, diluted with 2 ml.

H2O, and extracted with AcOEt. The organic extract was evaporated to dryness and the

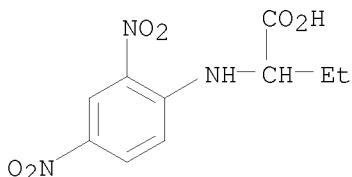
residue subjected to thinlayer chromatography on silica gel, using Et2O for development. An aliquot of the eluate was used to determine 4-androstene-3,17-dione (II) by a micro-Zimmermann reaction. Rf values of I and other 17-keto steroids and II and other oxidation products are tabulated to show that a satisfactory separation was achieved. It was shown by experiment that 11-oxo steroids did not interfere. The precision of the method was calculated by the formula of Snedecor (Biometrics 8, 85(1952)) to be about 2  $\gamma$  when perfect thin-layer chromatograms were obtained. The sensitivity was estimated to be about 4  $\gamma$ /24 hrs. Tables are presented showing the excretion of I by normal and unhealthy male (12) and female (5) patients.

IT 31356-29-3

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 76 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1963:404679 HCPLUS

DOCUMENT NUMBER: 59:4679

ORIGINAL REFERENCE NO.: 59:896b-d

TITLE: Thin-layer chromatographic detection of amino acids in urine

AUTHOR(S): Walz, D.; Fahmy, A. R.; Pataki, G.; Niederwieser, A.; Brenner, M.

CORPORATE SOURCE: Univ. Basel, Switz.

SOURCE: Experientia (1963), 19, 213-17

CODEN: EXPEAM; ISSN: 0014-4754

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Dinitrophenyl derivs. (I) of urinary amino acids are prepared by the method of Peraino and Harper (CA 56, 6285b). The excess reagent is extracted with ether, dried over anhydrous Na2SO4, and evaporated under vacuum. The residue is

taken up in acetone. Ether-soluble I is extracted following acidification with 6N HCl. Acidsol. I is then extracted with a mixture of equal parts of EtOAc and

BuOH. Following drying over anhydrous Na2SO4, the solvent is removed under vacuum and the residue taken up in a small quantity of EtOAc-BuOH. Plates

for chromatog. are prepared according to Brenner, et al. (CA 55, 20077b). Chromatograms are developed with toluene-2-chloroethanol pyridine-25% NH4OH (50:35:15:7 volume/volume); CHCl3-benzyl alc.-AcOH (70:30:3 volume/volume); CHCl3-MeOH-AcOH (70:30:5 volume/volume); CHCl3-MeOH-AcOH (95:5:1 volume/volume); pyridine; BuOH saturated with 25% NH4OH at room temperature The detection of

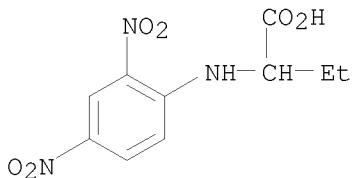
35

urinary constituents by multiple development and 2-dimensional chromatog. is described.

IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)-  
(detection of, in urine)

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 77 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1963:404678 HCAPLUS

DOCUMENT NUMBER: 59:4678

ORIGINAL REFERENCE NO.: 59:896a-b

TITLE: Two new staining procedures for quantitative estimation of proteins on electrophoretic strips

AUTHOR(S): Groth, S. Fazekas de St.; Webster, R. G.; Datyner, A.

CORPORATE SOURCE: Australian Natl. Univ., Canberra

SOURCE: Biochimica et Biophysica Acta (1963), 71, 377-91

CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

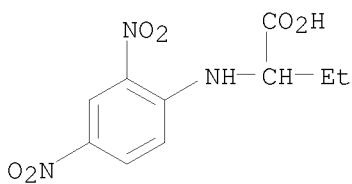
AB Two new procedures are described for the estimation of protein by direct photometry on electrophoretic strips. The protein complexes of Procion Brilliant Blue RS and Coomassie Brilliant Blue R250 are shown to follow Beer's law up to 50 and 20  $\gamma/cm.$ , resp. The lower limits of detection are 2 and 0.5  $\gamma/cm.$  Within these ranges the absolute amount of protein can be estimated within a single test with an error of about  $\pm 10\%$ . The major contribution to the error arises from uneven application of the samples. Relative concns. within a mixture of proteins can be evaluated to an error of less than  $\pm 3\%$ . Technical details of the procedures and of the equipment required are given in full, and their areas of usefulness discussed.

IT 31356-29-3

(Derived from data in the 7th Collective Formula Index (1962-1966))

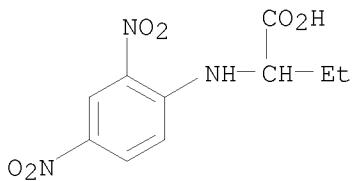
RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



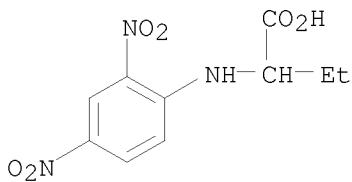
OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L11 ANSWER 78 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1962:404225 HCAPLUS  
 DOCUMENT NUMBER: 57:4225  
 ORIGINAL REFERENCE NO.: 57:941h-i,942a-b  
 TITLE: Spectrometric evaluation of the approximate pK of the carboxyl group in 2,4-dinitrophenyl amino acids  
 AUTHOR(S): Ramachandran, L. K.; Sastry, L. V. S.  
 CORPORATE SOURCE: Indian Inst. Sci., Bangalore, India  
 SOURCE: Biochemistry (1962), 1(1), 75-8  
 CODEN: BICBWA; ISSN: 0006-2960  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The changes in absorption at 360 m $\mu$  of 21 2,4-dinitrophenylamino acids at various hydrogen ion concns. were examined, and the approx. pK of the carboxyl group in many of these compds. was evaluated from a curve relating absorbancy to pH. The effect of the ionization of the carboxyl on the contribution of absorbancy at 360 m $\mu$  by the 2,4-dinitrophenyl (DNP) amino-chromophore was highly dependent on the distance of the carbon carrying the chromophore system from the carboxyl group. When this distance exceeded three C atoms, carboxyl ionization had little effect on absorbancy. The observed changes in the spectra would be consistent with resonance stabilization of the anion. DNP derivs. of  $\beta$ -aminobutyric acid, DL- $\alpha$ -aminobutyric acid,  $\beta$ -aminoisobutyric acid, and DL-isoserine were prepared and m. 166-8, 190, 154, and 145-8°, resp. The DNP derivative of DL-isoserine seemed to undergo a structural transformation at acid pH, probably due to elimination of one mole of water, which was reversible on increasing the pH.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)-  
 (ionization and spectrum of)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 79 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1962:49552 HCAPLUS  
 DOCUMENT NUMBER: 56:49552

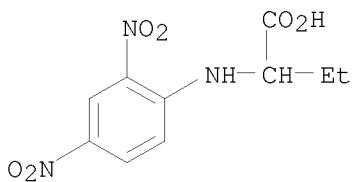
ORIGINAL REFERENCE NO.: 56:9391a-b  
 TITLE: Standard ionophoretic mobilities of various biochemicals, in amaranth units, at several pH values from 3.3 to 9.3  
 AUTHOR(S): Thornburg, W. W.; Werum, L. N.; Gordon, H. T.  
 CORPORATE SOURCE: California Packing Corp., Emeryville  
 SOURCE: Journal of Chromatography (1961), 6, 131-41  
 CODEN: JOCRAM; ISSN: 0021-9673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. CA 54, 19089f. The "Am value," defined as 0.01 of the distance between spots of the uncharged dye, Apolon, and the neg. charged dye, Amaranth, is tabulated for numerous known organic compds. (including N bases, amino acids, carbohydrates, organic acids, and phosphate esters) in 30% HCONH<sub>2</sub> organic buffers at 8 pH values ranging from 3.3 to 9.3. The pK and mol.-weight values calculable from ionophoretic data sometimes differ considerably from expected values owing to unusually strong mol. interactions with the buffers. The mobility pH pattern nevertheless gives significant information about mol. structure of unknowns.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)- (electrophoresis of)  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 80 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1961:106464 HCAPLUS  
 DOCUMENT NUMBER: 55:106464  
 ORIGINAL REFERENCE NO.: 55:20077b-c  
 TITLE: Thin-layer chromatography of amino acid derivatives on silica-gel G. N-(2,4-Dinitrophenyl) amino acids and 3-phenyl-2-thiohydantoins  
 AUTHOR(S): Brenner, M.; Niederwieser, A.; Pataki, G.  
 CORPORATE SOURCE: Univ. Basel, Switz.  
 SOURCE: Experientia (1961), 17, 145-53  
 CODEN: EXPEAM; ISSN: 0014-4754  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. Brenner and Niederwieser, CA 55, 4685e. The title compds. (I) and (II), resp., were separated by thin-layer chromatog. on silica-gel G. Acid- and H<sub>2</sub>O-soluble I were chromatographed in one dimension with PrOH:NH<sub>3</sub> (70:30). I not soluble in acid were separated 2-dimensionally; the 1st solvent-system was toluene, pyridine, ethylenechlorohydrin, 0.8N NH<sub>3</sub> (100:30:60:60), applied on equilibrated layers; the 2nd system was CHCl<sub>3</sub>, benzyl alc., AcOH (70:30:3). 39 refs.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)- (chromatog. of)

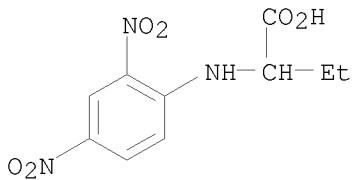
## STN Search

RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)

L11 ANSWER 81 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1961:106463 HCAPLUS  
 DOCUMENT NUMBER: 55:106463  
 ORIGINAL REFERENCE NO.: 55:20077a-b  
 TITLE: A simple spectrophotometric method for the determination of urea in blood and urine  
 AUTHOR(S): With, T. K.; Petersen, Tove Dreyer; Petersen, Birgit  
 SOURCE: Journal of Clinical Pathology (1961), 14, 202-4  
 CODEN: JCRAAK; ISSN: 0021-9746  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The method of Watt and Chrisp (CA 48, 6920b) for the determination of urea in pure solns. was modified to permit the determination of urea in blood and urine. The method is suitable for routine clin. analyses of large nos. of samples, except those from patients receiving sulfonamides or p-amino-salicylic acid. In these samples an atypical color reaction develops.  
 IT 31356-29-3  
 (Derived from data in the 6th Collective Formula Index (1957-1961))  
 RN 31356-29-3 HCAPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 82 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1961:71100 HCAPLUS  
 DOCUMENT NUMBER: 55:71100  
 ORIGINAL REFERENCE NO.: 55:13528i,13529a  
 TITLE: Separation of 2,4-dinitrophenyl derivatives of some amino acids by the countercurrent method of partitioning  
 AUTHOR(S): Khokhlov, A. S.; Ch'ih, Ch'ang-Ching

CORPORATE SOURCE: Inst. Antibiotics, Moscow  
 SOURCE: Biokhimiya (Moscow) (1960), 25, 1030-34  
 CODEN: BIOHAO; ISSN: 0320-9725

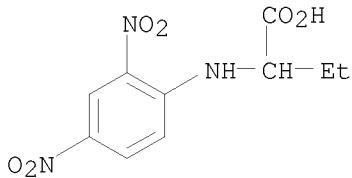
DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB The method of countercurrent partitioning was used for dinitrophenyl derivs. Low concns. of the components was art essential requisite. Accuracy of the method was sufficiently adequate for all practical purposes.

IT 31356-29-3P, Butyric acid, 2-(2,4-dinitroanilino)-  
 RL: PREP (Preparation)  
 (separation by countercurrent partition)

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 83 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1961:71099 HCAPLUS

DOCUMENT NUMBER: 55:71099

ORIGINAL REFERENCE NO.: 55:13528i

TITLE: Modification of the alcohol dehydrogenase (ADH) method in the determination of blood alcohol

AUTHOR(S): Alha, Antti R.; Tamminen, Veikko

CORPORATE SOURCE: Univ. Helsinki

SOURCE: Annales Medicinae Experimentalis et Biologiae Fenniae (1960), 38, 121-5

CODEN: AMEBA7; ISSN: 0003-4479

DOCUMENT TYPE: Journal

LANGUAGE: English

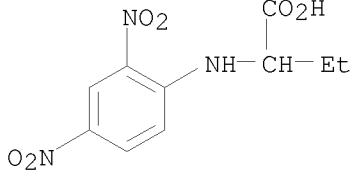
AB A modification of the ADH method is presented. EtOH is allowed to diffuse in enzyme solution using a Widmark flask at room temperature

IT 31356-29-3

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)

L11 ANSWER 84 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1961:13427 HCPLUS  
DOCUMENT NUMBER: 55:13427  
ORIGINAL REFERENCE NO.: 55:2649h-i,2650a-h  
TITLE: Synthesis of dinitrobenzomorpholines and a new ring system, triazolobenzomorpholine  
AUTHOR(S): Jurgens, Harold R.; Burton, Anne L.; Eichenbaum, Alice; Clapp, Leallyn B.  
CORPORATE SOURCE: Brown Univ., Providence, RI  
SOURCE: Journal of Organic Chemistry (1960), 25, 1710-13  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
OTHER SOURCE(S): CASREACT 55:13427  
AB Picramides (and related compds.) of  $\beta$ -amino alcs. in which there were bulky groups on the  $\alpha$ -C underwent ring closure with various bases to give substituted benzomorpholines. A nitro group in position 5 was reduced to an amine; diazotization gave a new ring system, triazolobenzomorpholine. The picramides of ethanolamine, m. 109.5-10.5°; 2-amino-1-butanol, m. 90-2°; 1-amino-2-propanol, m. 132.5-3.5°; 2-amino-3-butanol, m. 100-2.5°; diethanolamine, m. 138-9.5°; and 1-amino-2-methyl-2-propanol, m. 160.6-1.6°, were prepared by standard procedures, except the last. Other picramides were not isolated but were used directly to prepare the corresponding benzomorpholine. Picryl chloride (60 g.) in 600 ml. MeOH refluxed 45 min. with 46.5 g. 2-amino-2-methyl-1-propanol, 30 g. NaOMe in 200 ml. MeOH added during 10 min., the mixture stirred 0.5 hr. at reflux, cooled, and the product removed, washed, and isolated gave 40.5-5.1 g. 5,7-dinitro-3,3-di-methylbenzomorpholine (I), m. 174.5-6.0° (C<sub>6</sub>H<sub>6</sub>). I took up the calculated amount of H (in the presence of PtO<sub>2</sub>) for 2 nitro groups, but the product decomposed in air and was not further characterized. I (31.1 g.) in 400 ml. 95% alc. and 200 ml. 28% NH<sub>4</sub>OH was stirred mechanically at 45-55° while a slow stream of H<sub>2</sub>S was introduced during 2.5 hrs., the solution cooled, and the product collected. Concentration of the filtrate gave 15.6 g. 7-nitro-5-amino-3,3-dimethylbenzomorpholine (II), m. 182.5-4.5° (decomposition); benzal derivative m. 160-3° (95% alc.); monoacetyl derivative m. 195-6.5°. II (5 g.) in 50 ml. 20% H<sub>2</sub>SO<sub>4</sub> treated during 10 min. at 0° with 1.7 g. NaNO<sub>2</sub> in 10 ml. H<sub>2</sub>O, the mixture stirred 15 min. at 0-10°, and the product isolated gave 4.9 g. 8-nitro-4,4-di-methyltriazolo[1,5,4-de]benzomorpholine (III), yellow needles, m. 151.5-3.5°. III (0.92 g.) in 30 ml. MeOH reduced with H at 1 atmospheric over 0.25 g. PtO<sub>2</sub> gave 0.5 g. 8-amino-4,4-di-methyltriazolo [1,5,4-de] benzomorpholine (IV), cubic crystals, m. 217.5-20.5°; benzoyl derivative m. 219.5-21.5°. 3,5-Dinitro-4-chlorobenzoic acid was obtained in 95% yield from p-ClC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H. The acid was converted to the amide, m. 186°, in 83% yield via the acid chloride, m. 58°. The amide (12.4 g.) heated with 12 g. P<sub>2</sub>O<sub>5</sub> 15 min. at 300-50° and the resultant nitrile distilled at 220-5°/15 mm. and recrystd. gave 5.5 g. 3,5-dinitro-4-chlorobenzonitrile (IV), m. 143-4.5° (MeOH). IV (3. g.) refluxed 0.5 hr. with 2.5 g. 2-amino-2-methyl-1-propanol in 60 ml. alc. and refluxed an addnl. 0.5 hr. with 1.6 g. NaOMe in 60 ml. MeOH gave 1.2 g. 5-nitro-7-cyano-3,3-dimethylbenzomorpholine, orange crystals, m.

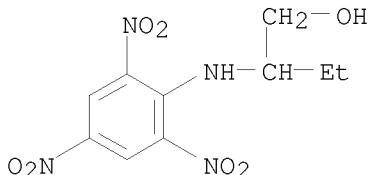
180-1.5°. The following compds. were similarly prepared:  
 3-hydroxymethyl-3-ethyl-5,7-dinitrobenzo-morpholine, orange crystals, m. 139.5-41°, 37%; 3-hydroxymethyl-3-methyl-5,7-dinitrobenzomorpholine, orange crystals, m. 147.2-8.6°, 47%; and 3,3-bis(hydroxymethyl)-5,7-dinitrobenzomorpholine, yellow powder, m. 158.5-60° (decomposition), 31%. Two nitro groups were best introduced into 4-chlorobenzotrifluoride, yielding 84% 3-nitro-4-chlorobenzotrifluoride and then 85% 3,5-dinitro-4-chlorobenzotrifluoride (VI). VI (7 g.) in 50 ml. MeOH refluxed with 4.65 g. 2-amino-2-methyl-1-propanol, 4 g. NaOMe added in 50 ml. MeOH, the mixture refluxed 10 min., and H<sub>2</sub>O added gave 4.8 g. 5-nitro-7-trifluoromethyl-3,3-dimethylbenzomorpholine (VII), golden needles, m. 108-9.5°. VII (1 g.) reduced quant. in 40 ml. MeOH at 1 atmospheric in 1 hr. over 0.3 g. PtO<sub>2</sub> and the product sublimed at 70°/1 mm. gave 0.8 g. 5-amino-7-trifluoromethyl-3,3-dimethylbenzomorpholine (VIII), m. 80-2°. VIII (0.27 g.) in 30 ml. 50% H<sub>2</sub>SO<sub>4</sub> treated during 10 min. with cold 0.12 g. NaNO<sub>2</sub> in 10 ml. H<sub>2</sub>O, the mixture poured into 100 ml. H<sub>2</sub>O, and the product recrystd. gave 0.10 g. 8-trifluoromethyl-4,4-di-methyltriazolo[1,5,4-de]benzomorpholine, m. 101-2.5° (dilute MeOH). Standard methods for diazotization of IV and coupling of the product with various compds. in NaOAc solution were used to obtain dyes as follows (coupling compound, m.p., color, % yield given): PhNMe<sub>2</sub>, 181-3°, orange-yellow, 76; PhNEt<sub>2</sub>, 149-51°, orange, 82; α-naphthylamine, 245-7°, dark red, 70; resorcinol, 225° (decomposition), orange-red, 20.

IT 103040-15-9P, 1-Butanol, 2-(2,4,6-trinitroanilino)-

RL: PREP (Preparation)  
 (preparation of)

RN 103040-15-9 HCPLUS

CN 1-Butanol, 2-[(2,4,6-trinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 85 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1957:86391 HCPLUS

DOCUMENT NUMBER: 51:86391

ORIGINAL REFERENCE NO.: 51:15685c

TITLE: Influence of buffers on the separation of dinitrophenyl derivatives of amino acids by means of paper chromatography

AUTHOR(S): Iwainsky, H.

CORPORATE SOURCE: Humboldt-Univ., Berlin

SOURCE: Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1954), 297, 194-8

CODEN: HSZPAZ; ISSN: 0018-4888

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The influence of various buffers on the paper chromatographic separation of

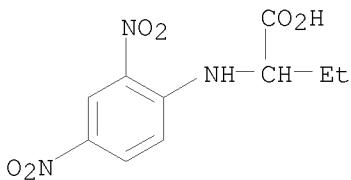
dinitrophenyl derivs. of amino acids (i.e. of cystine, asparagine, etc.) with various solvents is studied. The pH zone 9-11 is recommended as most suitable. BuOH-iso-AmOH-EtOH-buffer (20:20:6.5:30) is used as a new solvent mixture

IT 31356-29-3

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 31356-29-3 HCAPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 86 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1957:86390 HCAPLUS

DOCUMENT NUMBER: 51:86390

ORIGINAL REFERENCE NO.: 51:15684h-i,15685a-c

TITLE: Some cellulose ion exchangers of low substitution and their chromatographic application

AUTHOR(S): Porath, Jerker

CORPORATE SOURCE: Univ. Uppsala, Swed.

SOURCE: Arkiv foer Kemi (1957), 11, 97-106

CODEN: ARKEAD; ISSN: 0365-6128

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 50, 7204e.  $\text{CH}_2\text{Cl}_2$  (2 moles) in 200 ml. of EtOH and  $\text{Na}_2\text{SO}_3$  (1 mole) in 300 ml. of water were heated to  $120^\circ$  for 6 hrs. with stirring in an autoclave. The reaction mixture was evaporated to dryness, ground, and extracted continuously with boiling MeOH. The cooled extract gave

70

g. of  $\text{ClCH}_2\text{SO}_3\text{Na}$  (I). Cellulose powder (100 g.) and a solution of 200 g. of NaOH in 300 ml. of water was stirred and allowed to swell for 4-12 hrs. A solution of 10 g. of I in 60 ml. of water was added portion-wise with stirring. The mass was dried at  $90-5^\circ$  until 80% of the water was removed. The product should contain from 0.85 to 0.5 meq. of sulfonate groups per g. of dry powder; if lower, heat the mixture until the water content is reduced to 14%. Cool the mixture and pour into 1 l. of 95% EtOH, add 1 l. of N HCl slowly with stirring and cooling and allow to settle. Repeat the acid treatment, collect the ion exchanger (II) on a Buchner funnel, wash with 1 l. of 0.5N HCl, wash with water until neutral, and suck dry. Suspend II in water or buffer and mix thoroughly before packing in a column. Equine antidiiphtheria was separated into 4 components by using a column of II eluted with increasing concns. of phosphate buffer.

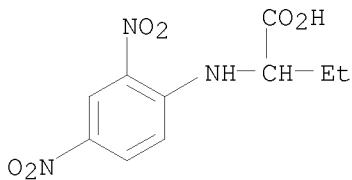
Sulfoethyl cellulose was prepared in the same way. Triethylaminoethyl cellulose (III) was prepared by heating 80 g. of diethylaminoethyl cellulose with 350 ml. of 10% EtBr in EtOH for 4 hrs. (C.A. 44, 11104a). III-Br is stored wet or dry. III-OH is prepared by washing III-Br successively with 1 l. of 1% aqueous NaOH, distilled water to neutrality,  $\text{Me}_2\text{CO}$ , and  $\text{Et}_2\text{O}$ .

IT 31356-29-3

(Derived from data in the 6th Collective Formula Index (1957-1961))

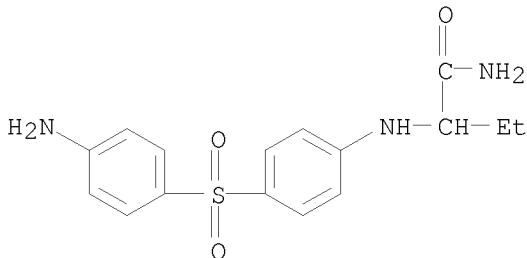
STN Search

RN 31356-29-3 HCAPLUS  
CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



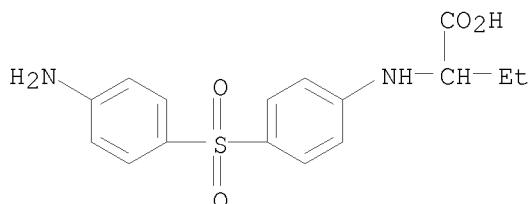
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L11 ANSWER 87 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1956:64344 HCAPLUS  
DOCUMENT NUMBER: 50:64344  
ORIGINAL REFERENCE NO.: 50:11966e-f  
TITLE: Studies in potential antimycobacterial agents. XII.  
Synthesis of some 4-hydroxy-3-quinolylhydrazine  
derivatives and their in vitro activity  
AUTHOR(S): Popli, S. P.; Vora, V. C.  
CORPORATE SOURCE: Central Drug Research Inst., Lucknow  
SOURCE: Journal of Scientific & Industrial Research (1955),  
14C, 228-30  
CODEN: JSIRAC; ISSN: 0022-4456  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB Some new 4-hydroxyquinolyl derivs. have been prepared and tested for in  
vitro tuberculostatic action.  
IT 873997-64-9P, Butyramide, 2-p-sulfanilylanilino-  
RL: PREP (Preparation)  
(preparation of)  
RN 873997-64-9 HCAPLUS  
CN Butanamide, 2-[(4-[(4-aminophenyl)sulfonyl]phenyl)amino]- (CA INDEX NAME)



L11 ANSWER 88 OF 94 HCAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1956:64343 HCAPLUS  
DOCUMENT NUMBER: 50:64343  
ORIGINAL REFERENCE NO.: 50:11966b-f  
TITLE: Studies in potential antimycobacterial agents. XI.  
Synthesis of p-amino-p'-(carboxyalkylamino)diphenyl

AUTHOR(S): sulfones, their esters, hydrazides, and amides  
 Khosla, M. C.; Anand, Nitya; Dhar, M. L.  
 CORPORATE SOURCE: Central Drug Research Inst., Lucknow  
 SOURCE: Journal of Scientific & Industrial Research (1955),  
 14C, 222-7  
 CODEN: JSIRAC; ISSN: 0022-4456  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB [In the following R1 = CO<sub>2</sub>Et, R2 = CO<sub>2</sub>Bu, R3 = CO<sub>2</sub>C<sub>8</sub>H<sub>17</sub>, R4 = CONHNH<sub>2</sub>, R5 = CONH<sub>2</sub>, R6 = CO<sub>2</sub>H.] A description is given of the synthesis of some 4-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NHR-4 (I), where R = carboxyalkyl, and their esters, hydrazides, and amides from 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SC<sub>6</sub>H<sub>4</sub>N(SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4)R-4 (II, R = K) and the esters of Br-substituted acids in anhydrous dioxane by standard methods.  
 The following II were prepared (R and m.p. given): CH<sub>2</sub>R<sub>1</sub>, 64°; CHMeR<sub>1</sub>, -; CHEtR<sub>1</sub>, 86°; CHBuR<sub>1</sub>, -; (CH<sub>2</sub>)<sub>5</sub>R<sub>1</sub>, 55°; (CH<sub>2</sub>)<sub>10</sub>R<sub>1</sub>, - . 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>N(SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4)R-4: were CH<sub>2</sub>R<sub>1</sub>, 168°; CHMeR<sub>1</sub>, 160°; CHBuR<sub>1</sub>, 130°; (CH<sub>2</sub>)R<sub>1</sub>, 95-6°; (CH<sub>2</sub>)<sub>10</sub>R<sub>1</sub>, 65°. 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NHR-4: CH<sub>2</sub>R<sub>1</sub>, 180°; CHMeR<sub>1</sub>, 115-16°; CHEtR<sub>1</sub>, 105°; CHBuR<sub>1</sub>, 91-2°; (CH<sub>2</sub>)<sub>5</sub>R<sub>1</sub>, 132-3°; (CH<sub>2</sub>)<sub>10</sub>R<sub>1</sub>, 90°. I: CH<sub>2</sub>R<sub>1</sub>, 179°; CHMeR<sub>1</sub>, 160°; CHEtR<sub>1</sub>, 102-4°; CHBuR<sub>1</sub>, 130°; (CH<sub>2</sub>)<sub>5</sub>R<sub>1</sub>, 147-9°; (CH<sub>2</sub>)<sub>10</sub>R<sub>1</sub>, 125°; CH<sub>2</sub>R<sub>2</sub>, 110°; CHMeR<sub>2</sub>, -; CHEtR<sub>2</sub>, 159-160°, 122-3°; (CH<sub>2</sub>)<sub>5</sub>R<sub>2</sub>, 108-9°; CH<sub>2</sub>R<sub>3</sub>, 115°; CHMeR<sub>3</sub>, -; CHEtR<sub>3</sub>, 93°; CHBuR<sub>3</sub>, 104-6°; (CH<sub>2</sub>)<sub>5</sub>R<sub>3</sub>, 115-17°; CH<sub>2</sub>R<sub>4</sub>, 180°; CHMeR<sub>4</sub>, 123-4°; CHBuR<sub>4</sub>, 173°; (CH<sub>2</sub>)<sub>5</sub>R<sub>4</sub>, 164-6°; (CH<sub>2</sub>)<sub>10</sub>R<sub>4</sub>, 148-9°; CH<sub>2</sub>R<sub>5</sub>, 248°; CHEtR<sub>5</sub>, 218-20°; CHBuR<sub>5</sub>, 202-3°; (CH<sub>2</sub>)<sub>5</sub>R<sub>5</sub>, -; (CH<sub>2</sub>)<sub>10</sub>R<sub>5</sub>, -; CH<sub>2</sub>R<sub>6</sub>, 188-90°; (CH<sub>2</sub>)<sub>10</sub>R<sub>6</sub>, 174-5°.  
 IT 873998-11-9, Butyric acid, 2-p-sulfanilylanilino-  
 RL: PREP (Preparation)  
 (and derivs.)  
 RN 873998-11-9 HCPLUS  
 CN Butanoic acid, 2-[(4-[(4-aminophenyl)sulfonyl]phenyl)amino]- (CA INDEX  
 NAME)



L11 ANSWER 89 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1956:20593 HCPLUS  
 DOCUMENT NUMBER: 50:20593  
 ORIGINAL REFERENCE NO.: 50:4279c  
 TITLE: Separation of dinitrophenols from dinitrophenyl  
 derivatives of amino acids and peptides  
 AUTHOR(S): Turba, F.; Gundlach, G.  
 SOURCE: Biochemische Zeitschrift (1955), 326, 322-4

CODEN: BIZEA2; ISSN: 0366-0753

DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB With anionotropic Al2O3 it was possible to sep. dinitrophenyl (DNP) derivs. of amino acids and peptides from dinitrophenol, which occurs in the production of the DNP derivs. and which interferes with the determination of free

amino groups of DNP derivs. of amino acids and peptides.

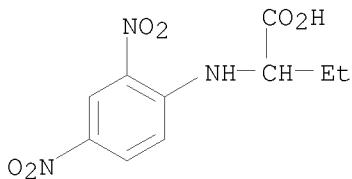
IT 31356-29-3P, Butyric acid, 2-(2,4-dinitroanilino)-

RL: PREP (Preparation)

(separation of mixts. containing dinitrophenol and)

RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



L11 ANSWER 90 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1955:46097 HCPLUS

DOCUMENT NUMBER: 49:46097

ORIGINAL REFERENCE NO.: 49:8859d-i, 8860a-b

TITLE: The applicability of reduction methods to the determination of terminal carboxyl amino acids in peptides and proteins

AUTHOR(S): Grassmann, Wolfgang; Hormann, Helmut; Endres, Horst

CORPORATE SOURCE: Max-Planck-Inst. Protein Leather Research, Regensburg, Germany

SOURCE: Chemische Berichte (1955), 88, 102-17

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 49:46097

AB cf. C.A. 49, 3816f, 7024b. The method was applied to synthetic peptides, which gave about 90% yield of N-dinitrophenylamino alc., from the terminal acid, and no reductive splitting of peptide bonds. Di-Me N-benzoyl-L-glutamate (0.8 g.) cooled and stirred with 3 g. LiBH4 in 30 cc. tetrahydrofuran, refluxed 30 hrs. in a dry atmospheric, cooled, 20 cc. H2O-saturated BuOH added, the filtrate evaporated in vacuo, the residue extracted with

Et2O, and the extract evaporated yielded 92.5% N-benzoyl-L-glutaminediol (I), white needles, m. 85°. I hydrolyzed 8 hrs. in 25% HCl, the BzOH filtered out, the filtrate evaporated in vacuo, the residue shaken 3 hrs. with 10 cc. H2O, 1 g. NaHCO3, and 0.8 g. 3,5-(O2N)2C6H3F (II) in 20 cc. EtOH, 0.2 g. glycine added to react with the excess II, H2O added, the EtOH evaporated, and the residue extracted with Et2O yielded 89.9% N-(3,5-dinitrophenyl)-L-glutaminediol (III), m. 103°, yellow needles from H2O. L-Lysine-2HCl, esterified in the cold with MeOH-HCl, the mixture evaporated, NaOMe in MeOH added, NaCl filtered out, and the product reduced with LiAlH4 and treated with II as above, yielded 51.4%

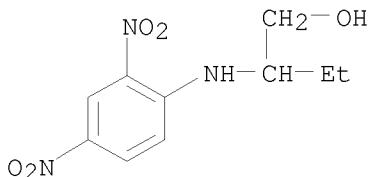
$\alpha, \epsilon$ -bis(3,5-dinitrophenyl)-L-lysinol (IV), fine bright yellow needles, m. 71° (from alc.-H<sub>2</sub>O). Similarly treated, Me N-benzoyl-DL-serinate (reduced with LiBH<sub>4</sub>) yielded 85.9% N-benzoyl-DL-serinol, m. 122°, fine white needles from Et<sub>2</sub>O, and 93.2% 3,5-dinitrophenyl-DL-serinol (V), fine yellow needles, m. 128° (from alc.-H<sub>2</sub>O). DL-Methionine esterified and acetylated in MeOH and AcOEt yielded 91.4% Me acetyl methionine, m. 96°, white leaflets which with LiBH<sub>4</sub> and II yielded 88.7% 3,5-dinitrophenyl-DL-2-aminobutanol (VI), m. 101° from alc.-H<sub>2</sub>O, identified with that prepared by treatment of DL-EtCH(NH<sub>2</sub>)CO<sub>2</sub>H with LiAlH<sub>4</sub> and II. Me aspartate was only partially reduced when treated as above with LiAlH<sub>4</sub> and II, yielding 69% 2,4 - (O<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>OCH:CHC(:CHOH)NHC<sub>6</sub>H<sub>3</sub>(NO<sub>2</sub>)<sub>2</sub> - 2,4 (VII), bright yellow needles from alc., which was proved to have 4 NO<sub>2</sub> groups (by titration with TiCl<sub>3</sub>) and a OH, and a CHO group. The terminal amino acids of the following synthetic peptides were determined by reduction of the ester with LiBH<sub>4</sub> and treatment with II as above, and the products identified by absorption spectra and R<sub>f</sub> value (peptide, product, yield given): glycyl-L-aspartic acid (the intermediate di-Me N-acetyl glycyl-L-aspartate, m. 107°), VII, 50%; L-valyl-glycyl-L-lysine, IV, 89.4%; glycyl-L-phenylalanyl-L-glutamic acid, III, 90.7%; glycyl-L-leucyl-L-glutamic acid, III, 87.2% [also some 3,5-dinitrophenylleucine (VIII)]; L-leucylglycylglycine, 3,5-dinitrophenylcolamine (IX), 90%, with some VIII. Without esterification, the single acids gave 1% dinitrophenyl derivative; di- and tripeptides, 1.76-6%; peptides containing phenylalanine, 8-11%. Insulin treated similarly, and chromatographed on kieselguhr-celite showed 2.39% dinitrophenylalaninol (X) per 100% amino acid, 2,4-dinitrophenol (XI), and VIII, without esterification, 0.482% X. Absorption spectra between 200 and 450 m $\mu$  are given for III, IV, V, VI, VII, IX, X, and N,O-bis(dinitrophenyl)tyrosinol (XII). The dinitrophenyl derivs. can be quantitatively separated by columnar chromatography. The following R<sub>f</sub> values for paper chromatography were developed with Decalin-10% AcOH-iso-AmOH-CH<sub>2</sub>C<sub>1</sub>CH<sub>2</sub>OH (9:6:6:2) and are compared with values in other solvents (loc. cit.): IV, 0.49; XII, 0.29; V, 0.41; VII, 0.47; III, 0.55; IX, 0.52; X, 0.71; 3,5-dinitrophenylprolinol, 0.83; XI, 0.82; VI, 0.85; 3,5-dinitrophenylvalinol, 0.87; 3,5-dinitrophenylphenylalaninol, 0.85; 3,5-dinitrophenylleucinol, 0.86; VIII, 0.90.

IT 521298-16-8P, 1-Butanol, 2-(2,4-dinitroanilino)-, DL-  
RL: PREP (Preparation)

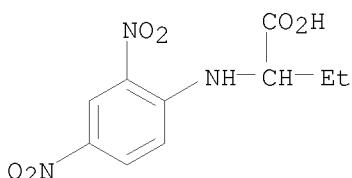
(preparation of)

RN 521298-16-8 HCAPLUS

CN 1-Butanol, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



ORIGINAL REFERENCE NO.: 49:4519i, 4520a-c  
 TITLE: A new sulfur-containing amino acid from subtilin  
 AUTHOR(S): Alderton, Gordon  
 CORPORATE SOURCE: Western Regional Research Lab., Albany, CA  
 SOURCE: Journal of the American Chemical Society (1953), 75, 2391-2  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C.A. 46, 1979b. In addition to lanthionine, a 2nd amino acid was isolated from the HCl hydrolyzates of subtilin. Its proposed structure is one of the  $\alpha$ -amino- $\beta$ -(2-amino-2-carboxyethylmercapto)-butyric acids. The configurations at the 2  $\alpha$ -C atoms were determined L-Methionine by a modification of the method of Fonken and Mozingo (C.A. 41, 4452d) yielded 57% L- $\alpha$ -aminobutyric acid (I),  $[\alpha]D24$  19.6° (c 5.00, 6N HCl). I by the method of Porter and Sanger (C.A. 42, 6920i) yielded DNP-L- $\alpha$ -aminobutyric acid (II),  $[\alpha]D26$  -38.0° (c 0.991, EtOAc),  $[\alpha]D27$  98.7° (c 0.62, 0.62% NaHCO<sub>3</sub>), 95° in white light. L-Cysteine-HCl with Raney Ni yielded L-alanine (III),  $[\alpha]D24$  13.6° (c 5.00, 0.999N HCl), which gave (dinitrophenyl)-L-alanine (IV),  $[\alpha]D27$  -11° (c 0.99, EtOAc),  $[\alpha]D27$  136° (c 1.02, 1.02% NaHCO<sub>3</sub>), 133.4° (white light). The new amino acid treated with Raney Ni and the product chromatographed yielded I and III (D-form), which gave II,  $[\alpha]W25$  116° (white light, c 0.519, 1% NaHCO<sub>3</sub>), and IV (D-form),  $[\alpha]W25$  -81° (white light, c 0.725, 1% NaHCO<sub>3</sub>). The new amino acid showed  $[\alpha]D24$  -34.7° (c 5.40, 1.01N HCl).  
 IT 31356-29-3P, Butyric acid, 2-(2,4-dinitroanilino)-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 31356-29-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)

L11 ANSWER 92 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1955:15700 HCPLUS  
 DOCUMENT NUMBER: 49:15700  
 ORIGINAL REFERENCE NO.: 49:3009h-i, 3010a-d  
 TITLE: Preparation and properties of  
 2,4-dinitrophenyl-L-amino acids  
 AUTHOR(S): Rao, Krishnarau R.; Sober, Herbert A.  
 CORPORATE SOURCE: Natl. Inst. of Health, Bethesda, MD  
 SOURCE: Journal of the American Chemical Society (1954), 76, 1328-31  
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AB Crystalline 2,4-dinitrophenyl derivs. of amino acids were prepared. The purification

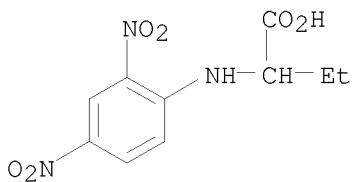
of many of the compds. required anhydrous conditions. The mol. rotations of the derivs. are 2 to 40 times those of the parent amino acid. UV absorption data and molar extinction values are given; the chromatog. behavior on paper in several solvent systems was examined. Phys. data concerning the derivs. are listed (amino acid, m.p. (°C.) (uncor.), [M]D24-6 (°) for N NaOH, 4% NaHCO<sub>3</sub>, AcOH, and shift in [M]D given): glycine, 203-4, -, -, -, -, -; L-alanine, 177, 367, -, 39, 335; β-alanine, 155-6, -, -, -, -, -; L-α-aminobutyric acid, 133, 266, 277, -23, 223; DL-α-aminobutyric acid, 143, -, -, -, -, -; γ-aminobutyric acid, 145-6, -, -, -, -, -; L-norvaline, 58-60, 170, -, -78, 129; L-valine, 132, 309, -, -79, 236; DL-valine, 184, -, -, -, -, -; L-isovaline, 141, 114, -, -, 88; L-leucine, 94-5, 177, 176, -135, 147; L-isoleucine, 113-14, 252, -, -104, 188; DL-isoleucine, 174-5, -, -, -, -, -; L-alloisoleucine, 119, 260, -, -119, 204; DL-alloisoleucine, 135-6, -, -, -; D-alloisoleucine, 146-7, -, -, -, -, -; L-α-aminononylic acid, 69-70, -277, -, -118, -, -335; L-serine, 173-4, -, 341, -65, 325; DL-serine, 200-2, -, -, -, -, -; L-threonine, 145, -, 305, -141, 341; DL-threonine, 178, -, -, -, -, -; L-allothreonine, 152, -, 305, -84, 260; DL-allothreonine, 133-4, -, -, -, -, -; γ-hydroxy-L-α-aminobutyric acid, 164-5, -, 75, -179, 61; ε-hydroxy-L-α-aminocaproic acid, 141-2, 119, -, -134, 72; DL-methionine, 117-18, -, -, -, -, -; DL-ethionine, 104-5, -, -, -, -; L-cystine (di), 109, -, -1487, -1833, -930; S-benzyl-L-cystine, 111, -, -, -669, -610; L-phenylalanine, 189, -310, -261, -342, -298; L-tyrosine (O, N, di), 178-82 (decomposition), -, -, -60, -42; L-tryptophan, 221 (decomposition), -1291, -, -672, -1222; L-proline, 138, -2172, -, -1978, -2080; DL-proline, 181, -, -, -, -; L-hydroxyproline, 174-5, -3852, -, -3410, -3751; L-allohydroxyproline, -, -2706, -1874, -1322, -2665; DL-pipecolic acid, 138-9, -, -, -, -, -; L-aspartic acid, 186-7, 275, -, -20, 241; L-glutamic acid, -, -20, -, -253, -67; DL-glutamic acid, 148-9, -, -, -, -, -; L-asparagine, 180-2, -, 190, -100, 98; L-glutamine, 189-91, -177, -172, -302, -157; L-α,γ-diaminobutyric acid (di), 120-2 (decomposition), -, -, -360, -398; L-ornithine (di), 156-7, -, -, -339, -377; L-lysine (di), 170-2 (decomposition), -, -, -127, -165; L-histidine, 232-4, -107, -, -, -, -119; L-arginine, 260, -, -, -121, -169

IT 31356-29-3P, Butyric acid, 2-(2,4-dinitroanilino)-, DL-

RL: PREP (Preparation)  
(preparation of)

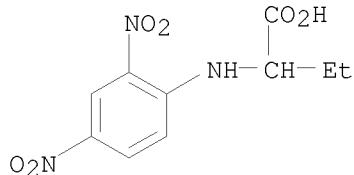
RN 31356-29-3 HCPLUS

CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD  
(6 CITINGS)

L11 ANSWER 93 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1955:3769 HCPLUS  
 DOCUMENT NUMBER: 49:3769  
 ORIGINAL REFERENCE NO.: 49:730f-g  
 TITLE: Photolysis of dinitrophenylamino acids  
 AUTHOR(S): Akabori, Shiro; Ikenada, Tokuji; Okada, Yoshimi;  
 Kohno, Keiichi  
 CORPORATE SOURCE: Osaka Univ.  
 SOURCE: Proceedings of the Japan Academy (1953), 29, 509-10  
 CODEN: PJACAW; ISSN: 0021-4280  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB Quant. studies of the photolysis of dinitrophenylamino acids (DNP-amino acids) revealed that the decrease in color is not proportional to the degree of decomposition. While  $\alpha$ -DNP-amino acids are photosensitive,  $\epsilon$ -mono-DNP-lysine is not. The velocities of the photodecompn. of DNP-alanine, -glycine, -valine, and -aspartic acid are similar.  
 IT 31356-29-3, Butyric acid, 2-(2,4-dinitroanilino)-  
 (photolysis of)  
 RN 31356-29-3 HCPLUS  
 CN Butanoic acid, 2-[(2,4-dinitrophenyl)amino]- (CA INDEX NAME)



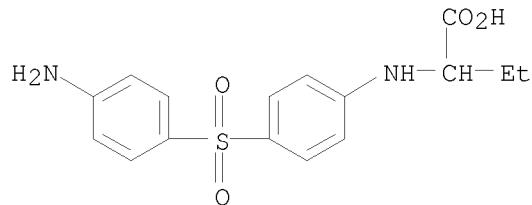
L11 ANSWER 94 OF 94 HCPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1953:12331 HCPLUS  
 DOCUMENT NUMBER: 47:12331  
 ORIGINAL REFERENCE NO.: 47:2207f-g  
 TITLE: Amino diphenyl sulfones  
 INVENTOR(S): Rawlins, Albert L.  
 PATENT ASSIGNEE(S): Parke, Davis & Co.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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AB US 2589211 19520318 US  
 (p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>SO<sub>2</sub>, RX, and EtOH refluxed 18-24 hrs. give  
 p-(p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>NHR (I), where R is a lower aliphatic carboxylic acid  
 or ester residue. Examples are given of I where R is: 2-carboxyethyl, m.  
 75°; carboxymethyl; 1-carboxypropyl; and 2-carboxypropyl. Other  
 similar products are mentioned. They are useful as antiseptics and  
 antibacterials. Cf. C.A. 43, 2637f.  
 IT 873998-11-9P, Butyric acid, 2-p-sulfanilylanilino-  
 RL: PREP (Preparation)  
 (preparation of)

STN Search

RN 873998-11-9 HCAPLUS  
CN Butanoic acid, 2-[[4-[(4-aminophenyl)sulfonyl]phenyl]amino]- (CA INDEX  
NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

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Updated Search